

# Approximate Nearest Neighbor Search in High Dimensions

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## Abstract

The nearest neighbor problem is defined as follows: Given a set  $P$  of  $n$  points in some metric space  $(X, D)$ , build a data structure that, given any point  $q$ , returns a point in  $P$  that is closest to  $q$  (its “nearest neighbor” in  $P$ ). The data structure stores additional information about the set  $P$ , which is then used to find the nearest neighbor without computing all distances between  $q$  and  $P$ . The problem has a wide range of applications in machine learning, computer vision, databases and other fields.

To reduce the time needed to find nearest neighbors and the amount of memory used by the data structure, one can formulate the *approximate* nearest neighbor problem, where the goal is to return any point  $p' \in P$  such that the distance from  $q$  to  $p'$  is at most  $c \cdot \min_{p \in P} D(q, p)$ , for some  $c \geq 1$ . Over the last two decades, many efficient solutions to this problem were developed. In this article we survey these developments, as well as their connections to questions in geometric functional analysis and combinatorial geometry.

## 1 Introduction

The *nearest neighbor* problem is defined as follows: Given a set  $P$  of  $n$  points in a metric space defined over a set  $X$  with distance function  $D$ , build a data structure<sup>1</sup> that, given any “query” point  $q \in X$ , returns its “nearest neighbor”  $\arg \min_{p \in P} D(q, p)$ . A particularly interesting and well-studied case is that of nearest neighbor in geometric spaces, where  $X = \mathbb{R}^d$  and the metric  $D$  is induced by some norm. The problem has a wide range of applications in machine learning, computer vision, databases and other fields, see [SDI06, AI08] for an overview.

A simple solution to this problem would store the set  $P$  in memory, and then, given  $q$ , compute all distances  $D(q, p)$  for  $p \in P$  and select the point  $p$  with the minimum distance. Its disadvantage is the computational cost: computing all  $n$  distances requires at least  $n$  operations. Since in many applications  $n$  can be as large as  $10^9$  (see e.g., [STS<sup>+</sup>13]), it was necessary to develop faster methods that find the nearest neighbors without explicitly computing all distances from  $q$ . Those methods compute and store additional information about the set  $P$ , which is then used to find nearest neighbors more efficiently. To illustrate this idea, consider another simple solution for the case where  $X = \{0, 1\}^d$ . In this case, one could precompute and store in memory the answers to all  $2^d$  queries  $q \in X$ ; given  $q$ , one could then return its nearest neighbor by performing only a single memory lookup. Unfortunately, this approach requires memory of size  $2^d$ , which again is inefficient ( $d$  is at least  $10^3$  or higher in many applications).

The two aforementioned solutions can be viewed as extreme points in a tradeoff between the time to answer a query (“query time”) and the amount of memory used (“space”)<sup>2</sup>. The study of this tradeoff dates back to the work of Minsky and Papert ([MP69], p. 222), and has become one of the key topics in the field of *computational geometry* [PS85]. During the 1970s and 1980s many efficient

<sup>1</sup>See Section 1.1 for a discussion about the computational model.

<sup>2</sup>There are other important data structure parameters, such as the time needed to construct it. For the sake of simplicity, we will mostly focus on query time and space.

solutions have been discovered for the case when  $(X, D) = (\mathbb{R}^d, \ell_2)$  and  $d$  is a constant independent of  $n$ . For example, for  $d = 2$ , one can construct a data structure using  $O(n)$  space with  $O(\log n)$  query time [LT80]. Unfortunately, as the dimension  $d$  increases, those data structures become less and less efficient. Specifically, it is known how construct data structures with  $O(d^{O(1)} \log n)$  query time, but using  $n^{O(d)}$  space ([Mei93], building on [Cla88]).<sup>3</sup> Furthermore, there is evidence that data structures with query times of the form  $n^{1-\alpha} d^{O(1)}$  for some constant  $\alpha > 0$  might be difficult to construct efficiently.<sup>4</sup>

The search for efficient solutions to the nearest neighbor problem has led to the question whether better space/query time bounds could be obtained if the data structure was allowed to report *approximate* answers. In the *c-approximate nearest neighbor* problem, the data structure can report any point  $p' \in P$  within distance  $c \cdot \min_{p \in P} D(q, p)$  from  $q$ ; the parameter  $c \geq 1$  is called “approximation factor”. The work of Arya, Mount and Bern [AM93, Ber93] showed that allowing  $c > 1$  indeed leads to better data structures, although their solutions still retained exponential dependencies on  $d$  in the query time or space bounds [AM93] or required that the approximation factor  $c$  is polynomial in the dimension  $d$  [Ber93]. These bounds have been substantially improved over the next few years, see e.g., [Cla94, Cha98, AMN<sup>+</sup>98, Kle97] and the references therein.

In this article we survey the “second wave” of approximate nearest neighbor data structures, whose query time and space bounds are polynomial in the dimension  $d$ .<sup>5</sup> At a high level, these data structures are obtained in two steps. In the first step, the approximate *nearest* neighbor problem is reduced to its “decision version”, termed approximate *near* neighbor (see e.g. [HPIM12]). The second step involves constructing a data structure for the latter problem. In this survey we focus mostly on the second step.

The approximate near neighbor problem is parameterized by an approximation factor  $c > 1$  as well as a “scale parameter”  $r > 0$ , and defined as follows.

**Definition 1.1** (*(c, r)-Approximate Near Neighbor*). *Given a set  $P$  of  $n$  points in a metric space  $(X, D)$ , build a data structure  $\mathcal{S}$  that, given any query point  $q \in X$  such that the metric ball  $B_D(q, r) = \{p \in X : D(p, q) \leq r\}$  contains a point in  $P$ ,  $\mathcal{S}$  returns any point in  $B_D(q, cr) \cap P$ .*

Note that the definition does not specify the behavior of the data structure if the ball  $B_D(q, r)$  does not contain any point in  $P$ . We omit the index  $D$  when it is clear from the context.

The above definition applies to algorithms that are *deterministic*, i.e., do not use random bits. However, most of the approximate near neighbor algorithms in the literature are *randomized*, i.e., generate and use random bits while constructing the data structure. In this case, the data structure  $\mathcal{S}$  is a random variable, sampled from some distribution. This leads to the following generalization.

**Definition 1.2** (*(c, r,  $\delta$ )-Approximate Near Neighbor*). *Given a set  $P$  of  $n$  points in a metric space  $(X, D)$ , build a data structure  $\mathcal{S}$  that, given any query point  $q \in X$  such that  $B(q, r) \cap P \neq \emptyset$ ,*

$$\Pr_{\mathcal{S}}[\mathcal{S} \text{ returns any point in } B(q, cr) \cap P] \geq 1 - \delta$$

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<sup>3</sup>This exponential dependence on the dimension is due to the fact that those data structures compute and store the *Voronoi decomposition* of  $P$ , i.e., the decomposition of  $\mathbb{R}^d$  into cells such that all points in each cell have the same nearest neighbor in  $P$ . The combinatorial complexity of this decomposition could be as large as  $n^{\Omega(d)}$  [Car11].

<sup>4</sup>If such a data structure could be constructed in polynomial time  $n^{O(1)} d^{O(1)}$ , then the Strong Exponential Time Hypothesis [Wil18] would be false. This fact essentially follows from [Wil05], see the discussion after Theorem 1 in [APRS16].

<sup>5</sup>Due to the lack of space, we will not cover several important related topics, such as data structures for point-sets with low intrinsic dimension [Cla06], approximate furthest neighbor, approximate nearest line search [Mah14] and other variants of the problem.

The probability of failure  $\delta$  of the data structure can be reduced by independently repeating the process several times, i.e., creating several data structures. Therefore, in the rest of the survey we will set  $\delta$  to an arbitrary constant, say,  $1/3$ . We will use  $(c, r)$ -ANN to denote  $(c, r, 1/3)$ -Approximate Near Neighbor.

## 1.1 Computational model

For the purpose of this survey, a data structure of size  $M$  is an array  $A[1 \dots M]$  of numbers (“the memory”), together with an associated algorithm that, given a point  $q$ , returns a point in  $P$  as specified by the problem. The entries  $A[i]$  of  $A$  are called “memory cells”. Due to lack of space, we will not formally define other details of the computational model, in particular what an algorithm is, how to measure its running time, what is the range of the array elements  $A[i]$ , etc. There are several ways of defining these notions, and the material in this survey is relatively robust to the variations in the definitions. We note, however, that one way to formalize these notions is to restrict all numbers, including point coordinates, memory entries, etc, to rational numbers of the form  $a/b$ , where  $a \in \{-n^{O(1)} \dots n^{O(1)}\}$  and  $b = n^{O(1)}$ , and to define query time as the maximum number of memory cells accessed to answer any query  $q$ .

For an overview of these topics and formal definitions, the reader is referred to [Mil99]. For a discussion specifically geared towards mathematical audience, see [FK09].

## 2 Data-independent approach

The first approach to the approximate near neighbor problem has been via data-independent data structures. These are data structures where the memory cells accessed by the query algorithm do not depend on the data set  $P$ , but only on  $q$  and (for randomized data structures) the random bits used to construct the data structure. In this section, we describe two methods for constructing such data structures, based on *oblivious dimension-reduction*, and on *randomized space partitions*. These methods give ANN data structures for the  $\ell_1$  and  $\ell_2$  spaces in particular.

### 2.1 ANN via dimension reduction

As described in the introduction, there exist ANN data structures with space and query time at most exponential in the dimension  $d$ . Since exponential space/time bounds are unaffordable for large  $d$ , a natural approach is to perform a *dimension reduction* beforehand, and then solve the problem in the lower, reduced dimension. The main ingredient of such an approach is a map  $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$  that preserves distances up to a  $c = 1 + \varepsilon$  factor, where  $k = O(\log n)$ . Then a space bound exponential in  $k$  becomes polynomial in  $n$ .

Such dimension-reducing maps  $f$  indeed exist for the  $\ell_2$  norm if we allow randomization, as first shown in the influential paper by Johnson and Lindenstrauss:

**Lemma 2.1** ([JL84]). *Fix dimension  $d \geq 1$  and a “target” dimension  $k < d$ . Let  $A$  be the projection of  $\mathbb{R}^d$  to its  $k$ -dimensional subspace selected uniformly at random (with respect to the Haar measure), and define  $f : \mathbb{R}^d \rightarrow \mathbb{R}^k$  as  $f(x) = \frac{\sqrt{d}}{\sqrt{k}}Ax$ . Then, there is a universal constant  $C > 0$ , such that for any  $\varepsilon \in (0, 1/2)$ , and any  $x, y \in \mathbb{R}^d$ , we have that*

$$\Pr_A \left[ \frac{\|f(x) - f(y)\|}{\|x - y\|} \in (1 - \varepsilon, 1 + \varepsilon) \right] \geq 1 - e^{-C\varepsilon^2 k}.$$

We can now apply this lemma, with  $k = O\left(\frac{\log n}{\varepsilon^2}\right)$ , to a set of points  $P$  to show that the map  $f$  has a  $(1 + \varepsilon)$  distortion on  $P$ , with probability at least  $2/3$ . Most importantly the map  $f$  is “oblivious”, i.e., it does not depend on  $P$ .

We now show how to use Lemma 2.1 to design a  $(1 + O(\varepsilon), r)$ -ANN data structure with the following guarantees.

**Theorem 2.2** ([IM98, HPIM12]). *Fix  $\varepsilon \in (0, 1/2)$  and dimension  $d \geq 1$ . There is a  $(1 + O(\varepsilon), r)$ -ANN data structure over  $(\mathbb{R}^d, \ell_2)$  achieving  $Q = O(d \cdot \frac{\log n}{\varepsilon^2})$  query time, and  $S = n^{O(\log(1/\varepsilon)/\varepsilon^2)} + O(d(n + k))$  space. The time needed to build the data structure is  $O(S + ndk)$ .*

*Proof sketch.* First, assume there is a  $(1 + \varepsilon, r)$ -ANN data structure  $\mathcal{A}$  for the  $k$ -dimensional  $\ell_2$  space, achieving query time  $Q(n, k)$  and space bounded by  $S(n, k)$ . For  $k = O(\frac{\log n}{\varepsilon^2})$ , we consider the map  $f$  from Lemma 2.1. For the dataset  $P$ , we compute  $f(P)$  and preprocess this set using  $\mathcal{A}$  (with the scale parameter  $r(1 + \varepsilon)$ ). Then, for a query point  $q \in \mathbb{R}^d$ , we query the data structure  $\mathcal{A}$  on  $f(q)$ . This algorithm works for a fixed dataset  $P$  and query  $q$  with  $5/6$  probability, by applying Lemma 2.1 to the points in the set  $P \cup \{q\}$ . The map  $f$  preserves all distances between  $P$  and  $q$  up to a factor of  $1 + \varepsilon$ .

We now construct  $\mathcal{A}$  with space  $S(n, k) = n \cdot (1/\varepsilon)^{O(k)}$  and  $Q(n, k) = O(k)$ , which yields the stated bound for  $k = O(\frac{\log n}{\varepsilon^2})$ . Given the scale parameter  $r$ , we discretize the space  $\mathbb{R}^k$  into cubes of sidelength  $\varepsilon r / \sqrt{k}$ , and consider the set  $S$  of cubes that intersect any ball  $B(p', r)$  where  $p' \in f(P)$ . Using standard estimates on the volume of  $\ell_2$  balls, one can prove that  $|S| \leq n \cdot (1/\varepsilon)^{O(k)}$ . The data structure then stores the set  $S$  in a dictionary data structure.<sup>6</sup> For a query  $f(q)$ , we just compute the cube that contains  $f(q)$ , and check whether it is contained in set  $S$  using the dictionary data structure. We note that there is an additional  $1 + \varepsilon$  factor loss from discretization since the diameter of a cube is  $\varepsilon r$ .  $\square$

A similar approach was introduced [KOR00] in the context of the Hamming space  $\{0, 1\}^d$ . An important difference is that there is no analog of Lemma 2.1 for the Hamming space [BC05].<sup>7</sup> Therefore, [KOR00] introduce a weaker notion of randomized dimension reduction, which works only for a *fixed scale*  $r$ .

**Lemma 2.3** ([KOR00]). *Fix the error parameter  $\varepsilon \in (0, 1/2)$ , dimension  $d \geq 1$ , and scale  $r \in [1, d]$ . For any  $k \geq 1$ , there exists a randomized map  $f : \{0, 1\}^d \rightarrow \{0, 1\}^k$  and an absolute constant  $C > 0$ , satisfying the following for any fixed  $x, y \in \{0, 1\}^d$ :*

- if  $\|x - y\|_1 \leq r$ , then  $\Pr_f[\|f(x) - f(y)\|_1 \leq k/2] \geq 1 - e^{-C\varepsilon^2 k}$ ;
- if  $\|x - y\|_1 \geq (1 + \varepsilon)r$ , then  $\Pr_f[\|f(x) - f(y)\|_1 > (1 + \varepsilon/2) \cdot k/2] \geq 1 - e^{-C\varepsilon^2 k}$ .

The map  $f$  can be constructed via a random projection over  $GF(2)$ . That is, take  $f(x) = Ax$ , where  $A$  is a  $k \times d$  matrix for  $k = O(\log(n)/\varepsilon^2)$ , with each entry being 1 with some fixed probability  $p$ , and zero otherwise. The probability  $p$  depends solely on  $r$ . The rest of the algorithm proceeds as before, with the exception that the “base” data structure  $\mathcal{A}$  is particularly simple: just store the answer for any dimension-reduced query point  $f(q) \in \{0, 1\}^k$ . Since there are only  $2^k = n^{O(1/\varepsilon^2)}$  such possible queries, and computing  $f(q)$  takes  $O(dk)$  time, we get the following result.

<sup>6</sup>In the dictionary problem, we are given a set  $S$  of elements from a discrete universe  $U$ , and we need to answer queries of the form “given  $x$ , is  $x \in S$ ?”. This is a classic data structure problem and has many solutions. One concrete solution is via a hashing [CLRS01], which achieves space of  $O(|S|)$  words, each of  $O(\log |U|)$  bits, and query time of  $O(1)$  in expectation.

<sup>7</sup>In fact, it has been shown that spaces for which analogs of Lemma 2.1 hold are “almost” Hilbert spaces [JN09].

**Theorem 2.4** ([KOR00]). *Fix  $\varepsilon \in (0, 1/2)$  and dimension  $d \geq 1$ . There is a  $(1 + O(\varepsilon), r)$ -ANN data structure over  $(\{0, 1\}^d, \ell_1)$  using  $n^{O(1/\varepsilon^2)} + O(d(n + k))$  space and  $O(d \cdot \frac{\log n}{\varepsilon^2})$  query time.*

As a final remark, we note we cannot obtain improved space bounds by improving the dimension reduction lemmas 2.1 and 2.3. Indeed the above lemmas are tight as proven in [JW13]. There was however work on improving the *run-time complexity* for computing a dimension reduction map, improving over the naïve bound of  $O(dk)$ ; see [AC09, DKS10, AL13, KW11, NPW14, KN14].

## 2.2 ANN via space partitions: Locality-Sensitive Hashing

While dimension reduction yields ANN data structure with polynomial space, this is not enough in applications, where one desires space as close as possible to linear in  $n$ . This consideration led to the following, alternative approach, which yields smaller space bounds, albeit at the cost of increasing the query time to something of the form  $n^\rho$  where  $\rho \in (0, 1)$ .

The new approach is based on randomized space partitions, and specifically on Locality-Sensitive Hashing, introduced in [IM98].

**Definition 2.5** (Locality-Sensitive Hashing (LSH)). *Fix a metric space  $(X, D)$ , scale  $r > 0$ , approximation  $c > 1$  and a set  $U$ . Then a distribution  $\mathcal{H}$  over maps  $h : X \rightarrow U$  is called  $(r, cr, p_1, p_2)$ -sensitive if the following holds for any  $x, y \in X$ :*

- if  $D(x, y) \leq r$ , then  $\Pr_h[h(x) = h(y)] \geq p_1$ ;
- if  $D(x, y) > cr$ , then  $\Pr_h[h(x) = h(y)] \leq p_2$ .

The distribution  $\mathcal{H}$  is called an LSH family, and has quality  $\rho = \rho(\mathcal{H}) = \frac{\log 1/p_1}{\log 1/p_2}$ .

In what follows we require an LSH family to have  $p_1 > p_2$ , which implies  $\rho < 1$ . Note that LSH mappings are also oblivious: the distribution  $\mathcal{H}$  does not depend on the point-set  $P$  or the query  $q$ .

Using LSH, [IM98] show how to obtain the following ANN data structure.

**Theorem 2.6** ([IM98]). *Fix a metric  $\mathcal{M} = (X, D)$ , a scale  $r > 0$ , and approximation factor  $c > 1$ . Suppose the metric admits a  $(r, cr, p_1, p_2)$ -sensitive LSH family  $\mathcal{H}$ , where the map  $h(\cdot)$  can be stored in  $\sigma$  space, and, for given  $x$ , can be computed in  $\tau$  time; similarly, assume that computing distance  $D(x, y)$  takes  $O(\tau)$  time. Let  $\rho = \rho(\mathcal{H}) = \frac{\log 1/p_1}{\log 1/p_2}$ . Then there exists a  $(c, r)$ -ANN data structure over  $\mathcal{M}$  achieving query time  $Q = O(n^\rho \cdot \tau \frac{\log_{1/p_2} n}{p_1})$  and space  $S = O(n^{1+\rho} \cdot \frac{1}{p_1} + n^\rho \frac{1}{p_1} \cdot \sigma \cdot \log_{1/p_2} n)$  (in addition to storing the original dataset  $P$ ). The time needed to build this data structure is  $O(S \cdot \tau)$ .*

While we describe some concrete LSH families later on, for now, one can think of the parameters  $\tau, \sigma$  as being proportional to the dimension of the space (although this is not always the case).

The overall idea of the algorithm is to use an LSH family as a pre-filter for the dataset  $P$ . In particular, for a random partition  $h$  from the family  $\mathcal{H}$ , the query point  $q$  will likely collide with its near neighbor (with probability at least  $p_1$ ), but with few points at a distance  $\geq cr$ , in expectation at most  $p_2 \cdot n$  of them. Below we show how an extension of this idea yields Theorem 2.6.

*Proof sketch.* Given an LSH family  $\mathcal{H}$ , we can build a new, derived LSH family via a certain tensoring operation. In particular, for an integer  $k \geq 1$ , consider a new distribution  $\mathcal{G}_k$  over maps  $g : X \rightarrow U$ , where  $g(\cdot)$  is obtained by picking  $k$  i.i.d. functions  $h_1, \dots, h_k$  chosen from  $\mathcal{H}$  and setting



$g(x) = (h_1(x), h_2(x), \dots, h_k(x))$ . Then, if  $\mathcal{H}$  is  $(r, cr, p_1, p_2)$ -sensitive,  $\mathcal{G}_k$  is  $(r, cr, p_1^k, p_2^k)$ -sensitive. Note that the parameter  $\rho$  of the hash family does not change, i.e.,  $\rho(\mathcal{G}_k) = \rho(\mathcal{H})$ .

The entire ANN data structure is now composed of  $L$  dictionary data structures (e.g., hash tables discussed in the previous section), where  $L, k \geq 1$  are parameters to fix later. The  $i$ -th hash table is constructed as follows. Pick a map  $g_i$  uniformly at random from  $\mathcal{G}_k$ , and store the set  $g_i(P)$  in the dictionary structure. At the query time, we iterate over  $i = 1 \dots L$ . For a given  $i$ , we compute  $g_i(q)$ , and use the dictionary structure to obtain the set of “candidate” points  $Q_i = \{p \in P : g_i(p) = g_i(q)\}$ . For each candidate point we compute the distance from  $q$  to that point. The process is stopped when all  $Q_i$ ’s are processed, or when a point within distance  $cr$  to  $q$  is found, whichever happens first.

To analyze the success probability, we note that the dictionary structure  $i$  succeeds if  $p^* \in Q_i$ , where  $p^*$  is the assumed point at distance at most  $r$  from  $q$ . This happens with probability at least  $p_1^k$ . Thus, we can take  $L = O(1/p_1^k)$  such dictionary structures, and thus guarantee success with a constant probability.

The expected query time is  $O(L(k\tau + Ln \cdot p_2^k \cdot \tau))$ , which includes both the computation of the maps  $g_1(q), \dots, g_L(q)$  and the of distances to the candidates in sets  $Q_1, \dots, Q_L$ . We can now derive the value of  $k$  that minimizes the above, obtaining  $k = \lceil \log_{1/p_2} n \rceil \leq \log_{1/p_2} n + 1$ , and hence  $L = O(n^\rho / p_1)$ .

Finally, note that the space usage is  $O(Ln)$  for the dictionary structures, plus  $O(Lk\sigma)$  for the description of the maps.  $\square$

## 2.3 Space partitions: LSH constructions

Theorem 2.6 assumes the existence of an LSH family  $\mathcal{H}$  with a parameter  $\rho < 1$ . In what follows we show a few examples of such families.

1. *Hamming space*  $\{0, 1\}^d$ , with  $\rho = 1/c$ . The distribution  $\mathcal{H}$  is simply a projection on a random coordinate  $i$ :  $\mathcal{H} = \{h_i : h_i(x) = x_i, i = 1, \dots, d\}$ . This family is  $(r, cr, 1 - r/d, 1 - cr/d)$ -sensitive, and hence  $\rho \leq 1/c$  [IM98].

This LSH scheme is near-optimal for the Hamming space, as described in Section 2.4. We also note that, since  $\ell_2$  embeds isometrically into  $\ell_1$  (see Section 6), this result extends to  $\ell_2$  as well.

2. *Euclidean space*  $(\mathbb{R}^d, \ell_2)$ , with  $\rho < 1/c$ . In [DIIM04], the authors introduced an LSH family which slightly improves over the above construction. It is based on random projections in  $\ell_2$ . In particular, define a random map  $h(x)$  as  $h(x) = \lfloor \frac{\langle x, g \rangle}{wr} + b \rfloor$ , where  $g$  is a random  $d$ -dimensional Gaussian vector,  $b \in [0, 1]$ , and  $w > 0$  is a fixed parameter. It can be shown that, for any fixed  $c > 1$ , there exists  $w > 0$  such that  $\rho < 1/c$ .
3. *Euclidean space*  $(\mathbb{R}^d, \ell_2)$ , with  $\rho \rightarrow 1/c^2$ . In [AI06], the authors showed an LSH family with a much better  $\rho$ , which later turned out to be optimal (see Section 2.4). At its core, the main idea is to partition the space into Euclidean balls.<sup>8</sup> It proceeds in two steps: 1) perform a random dimension reduction  $A$  to dimension  $t$  (a parameter), and 2) partition  $\mathbb{R}^t$  into balls. Since it is impossible to partition the space  $\mathbb{R}^t$  into balls precisely<sup>9</sup> when  $t \geq 2$ , instead one performs “ball carving”. The basic idea is to consider a sequence of randomly-centered balls

<sup>8</sup>In contrast, the above LSH family can be seen as partitioning the space into cubes: when considering the  $k$ -tensored family  $\mathcal{G} = \mathcal{H}^k$ , the resulting map  $g \in \mathcal{G}$  is equivalent to performing a random dimension reduction (by multiplying by a random  $k \times d$  Gaussian matrix), followed by discretization of the space into cubes.

<sup>9</sup>This is also termed *tessellation* of the space.

$B_1, B_2, \dots$ , each of radius  $wr$  for some parameter  $w > 1$ , and define the map  $h(x)$ , for  $x \in \mathbb{R}^d$ , to be the index  $i$  of the first ball  $B_i$  containing the point  $Ax$ . Since we want to cover an infinite space with balls of finite volume, the above procedure needs to be modified slightly to terminate in finite time. The modified procedure runs in time  $T = t^{O(t)}$ .

Overall, optimizing for  $w$ , one can obtain  $\rho = 1/c^2 + \frac{O(\log t)}{\sqrt{t}}$  which tends to  $1/c^2$  as  $t \rightarrow \infty$ . The time to hash is  $\tau = O(Tt + dt)$ , where  $T$  depends exponentially on the parameter  $t$ , i.e.,  $T = t^{\Theta(t)}$ . For the ANN data structure, the optimal choice is  $t = O(\log n)^{2/3}$ , resulting in  $\rho = 1/c^2 + \frac{O(\log \log n)}{(\log n)^{1/3}}$ .

The  $\ell_2$  LSH families can be extended to other  $\ell_p$ 's. For  $p < 1$ , [DIIM04] showed one can use method 2 as described above, but using  $p$ -stable distributions instead of Gaussians. See Section 6 for other extensions for  $p > 1$ .

We remark that there is a number of other widely used LSH families, including min-hash [Bro97, BGMZ97] and simhash [Cha02], which apply to different notions of similarity between points. See [AI08] for an overview.

## 2.4 Space partitions: impossibility results

It is natural to explore the limits of LSH families and ask what is the best  $\rho$  one can obtain for a given metric space as a function of the approximation  $c > 1$ . In [MNP07, OWZ14], it was proven that the LSH families [IM98, AI06] from the previous section are near-optimal: for the Hamming space, we must have  $\rho \geq 1/c - o(1)$ , and for the Euclidean space,  $\rho \geq 1/c^2 - o(1)$ . Below is the formal statement from [OWZ14].

**Theorem 2.7.** *Fix dimension  $d \geq 1$  and approximation  $c \geq 1$ . Let  $\mathcal{H}$  be a  $(r, cr, p_1, p_2)$ -sensitive LSH family over the Hamming space, and suppose  $p_2 \geq 2^{-o(d)}$ . Then  $\rho \geq 1/c - o_d(1)$ .*

Note that the above theorem also immediately implies  $\rho \geq 1/c^2 - o(1)$  for the Euclidean space, by noting that  $\|x - y\|_1 = \|x - y\|_2^2$  for binary vectors  $x$  and  $y$ .

Finally, we remark that some condition on  $p_2$  is necessary, as there exists an LSH family with  $p_2 = 0$ ,  $p_1 = 2^{-O(d)}$  and hence  $\rho = 0$ . To obtain the latter, one can use the “ball carving” family of [AI06], where the balls have radius  $wr = cr/2$ . Note however that such a family results in query time that is at least exponential in  $d$ , which LSH algorithms are precisely designed to circumvent.

## 3 (More) Deterministic algorithms

A drawback of data structures described in the previous section is that they allow “false negatives”: with a controllable but non-zero probability, the data structure can report nothing even if the ball  $B(q, r)$  is non-empty. Although most of the data structures described in the literature have this property, it is possible to design algorithms with stronger guarantees, including deterministic ones.

The first step in this direction was an observation (already made in [KOR00]) that for a finite metric  $(X, D)$  supported by  $(c, r)$ -ANN data structures, it is possible to construct a data structure that provides accurate answers to *all* queries  $q \in X$ . This is because one can construct and use  $O(\log |X|)$  independent data structures, reducing the probability of failure to  $\frac{1}{3^{|X|}}$ . By taking a union bound over all  $q \in X$ , the constructed data structure works, with probability at least  $2/3$ , for all queries  $X$ . Note that the space and query time bounds of the new data structure are  $O(\log |X|)$  times larger than the respective bounds for  $(c, r)$ -ANN. Unfortunately, the algorithm

for constructing such data structures has still a non-zero failure probability, and no deterministic polynomial-time algorithm for this task is known.

The first deterministic polynomial-time algorithm for constructing a data structure that works for all queries  $q \in X$  appeared in [Ind00a]. It was developed for  $d$ -dimensional Hamming spaces, and solved a  $(c, r)$ -ANN with an approximation factor  $c = 3 + \varepsilon$  for any  $\varepsilon > 0$ . The data structure had  $d(1/\varepsilon)^{O(1)}$  query time and used  $dn^{(1/\varepsilon)^{O(1)}}$  space. It relied on two components. The first component, “densification”, was a deterministic analog of the mapping in Lemma 2.3, which was shown to hold with  $k = (d/\varepsilon)^{O(1)}$ . Retrospectively, the mapping can be viewed as being induced by an adjacency matrix of an *unbalanced expander* [GUV09].

**Definition 3.1** (Expander). An  $(r, \alpha)$ -*unbalanced expander* is a bipartite simple graph  $G = (U, V, E)$ ,  $|U| = d, |V| = k$ , with left degree  $\Delta$  such that for any  $X \subset U$  with  $|X| \leq r$ , the set of neighbors  $N(X)$  of  $X$  has size  $|N(X)| \geq (1 - \alpha)\Delta|X|$ .

Given such a graph  $G$ , one can construct a mapping  $f = f_G : \{0, 1\}^d \rightarrow \Sigma^k$  for some finite alphabet  $\Sigma$  by letting  $f(x)_j$  to be the concatenation of all symbols  $x_i$  such that  $(i, j) \in E$ . Let  $H(x, y)$  be the Hamming distance between  $x$  and  $y$ , i.e., the number of coordinates on which  $x$  and  $y$  differ. We have that:

- $H(f(x), f(y)) \leq \Delta H(x, y)$ , since each difference between  $a$  and  $b$  contributes to at most  $\Delta$  differences between  $f(x)$  and  $f(y)$ . In particular  $H(f(x), f(y)) \leq \Delta r(1 - \varepsilon)$  if  $H(x, y) \leq r(1 - \varepsilon)$ .
- if  $H(x, y) \geq r$ , then  $H(f(x), f(y)) \geq (1 - \alpha)\Delta r$  (from the expansion property).

Thus, setting  $\alpha = \varepsilon/2$  yields guarantees analogous to Lemma 2.3, but using a deterministic mapping, and with coordinates of  $f(x)$  in  $\Sigma$ , not  $\{0, 1\}$ . To map into binary vectors, we further replace each symbol  $f(x)_j$  by  $C(f(x)_j)$ , where  $C : \Sigma \rightarrow \{0, 1\}^s$  is an *error-correcting code*, i.e., having the property that for any distinct  $a, b \in \Sigma$  we have  $H(C(a), C(b)) \in [s(1/2 - \varepsilon), s(1/2 + \varepsilon)]$ . We then use off-the-shelf constructions of expanders [GUV09] and codes [GRS14] to obtain the desired mapping  $g = C \circ f : \{0, 1\}^d \rightarrow \{0, 1\}^{ks}$ .

The second component partitions the coordinates of points  $g(x)$  into blocks  $S_1 \dots S_t$  of size  $\log(n)/\varepsilon^{O(1)}$  such that an analog of Lemma 2.3 holds for all projections  $g(x)_{S_l}$  and  $g(y)_{S_l}$  where  $x, y \in P$ ,  $l = 1 \dots t$ . Such a partitioning can be shown to exist using the probabilistic method, and can be computed deterministically in time polynomial in  $n$  via the method of conditional probabilities. Unfortunately, this property does not extend to the case where one of the points (say,  $x$ ) is a query point from  $X - P$ . Nevertheless, by averaging, there must be at least one block  $S_l$  such that  $H(g(x)_{S_l}, g(y)_{S_l}) \leq H(g(x), g(y))/t$ , where  $y$  is the nearest neighbor of  $x$  in  $P$ . It can be then shown that an approximate near neighbor of  $g(x)_{S_l}$  in  $\{g(y)_{S_l} : y \in P\}$  is an approximate nearest neighbor of  $x$  in  $P$ . Finding the nearest neighbor in the space restricted to a single block  $S_l$  can be solved via exhaustive storage using  $n^{1/\varepsilon^{O(1)}}$  space, as in Theorem 2.4.

Perhaps surprisingly, the above construction is the only known example of a polynomial-size deterministic approximate near neighbor data structure with a constant approximation factor. However, more progress has been shown for an “intermediary” problem, where the data structure avoids false negatives by reporting a special symbol  $\perp$ .

**Definition 3.2** ( $(c, r, \delta)$ -Approximate Near Neighbor Without False Negatives (ANNWFN)). *Given a set  $P$  of  $n$  points in a metric space  $(X, D)$ , build a data structure  $\mathcal{S}$  that, given any query point  $q \in X$  such that  $B(q, r) \cap P \neq \emptyset$ ,  $\mathcal{S}$  returns an element of  $(B(q, cr) \cap P) \cup \{\perp\}$ , and  $\Pr_{\mathcal{S}}[\mathcal{S} \text{ returns } \perp] \leq \delta$ .*



A  $(1 + \varepsilon, r, \delta)$ -ANNWFN data structure with bounds similar to those in Theorem 2.4 was given in [Ind00a]. It used densification and random block partitioning as described above. However, thanks to randomization, block partitioning could be assumed to hold even for the query point with high probability.

Obtaining “no false negatives” analogs of Theorem 2.2 turned out to be more difficult. The first such data structure was presented in [Pag16], for the Hamming space, achieving query time of the form (roughly)  $dn^{1.38/c}$ . Building on that work, very recently, Ahle [Ahl17] improved the bound to (roughly)  $dn^{1/c}$ , achieving the optimal runtime exponent.

In addition to variants of densification and random block partitioning, the latter algorithm uses a generalization of the space partitioning method from Section 2.2, called *locality sensitive filtering*. Such objects can be constructed deterministically in time and space roughly exponential in the dimension. Unfortunately, random block partitioning leads to blocks whose length is larger than  $\log n$  by at least a (large) constant, which results in large (although polynomial) time and space bounds. To overcome this difficulty, [Ahl17] shows how to combine filters constructed for dimension  $d$  to obtain a filter for dimension  $2d$ . This is achieved by using *splitters* [NSS95], which can be viewed as families of partitions of  $\{1 \dots 2d\}$  into pairs of sets  $(S_1, \overline{S_1}), (S_2, \overline{S_2}), \dots$  of size  $d$ , such that for any  $x, y$ , there is a pair  $(S_l, \overline{S_l})$  for which  $H(x_{S_l}, y_{S_l}) = H(x_{\overline{S_l}}, y_{\overline{S_l}}) \pm 1$ . The construction multiplies the space bound by a factor quadratic in  $d$ , which makes it possible to apply it a small but super-constant number of times to construct filters for (slightly) super-logarithmic dimension.

## 4 Data-dependent approach

In the earlier sections, we considered ANN data structures that are based on random and deterministic space partitions. The unifying feature of all of the above approaches is that the partitions used are independent of the dataset. This “data-independence” leads to certain barriers: for instance, the *best possible* LSH exponent is  $\rho \geq 1/c - o(1)$  for the  $\ell_1$  distance and  $\rho \geq 1/c^2 - o(1)$  for  $\ell_2$  (see Section 2.4). In this section, we show how to improve upon the above results significantly if one allows partitions to depend on the dataset.

This line of study has been developed in a sequence of recent results [AINR14, AR15, ALRW17]. However, even before these works, the data-dependent approach had been very popular in practice (see, e.g., surveys [WSSJ14, WLKC16]). Indeed, real-world datasets often have some implicit or explicit structure, thus it pays off to tailor space partitions to a dataset at hand. However, the theoretical results from [AINR14, AR15, ALRW17] improve upon data-independent partitions for *arbitrary* datasets. Thus, one must show that *any* set of  $n$  points has some structure that makes the ANN problem easier.

### 4.1 The result

In [AR15] (improving upon [AINR14]), the following result has been shown.

**Theorem 4.1.** *For every  $c > 1$ , there exists a data structure for  $(c, r)$ -ANN over  $(\mathbb{R}^d, \ell_2)$  with space  $n^{1+\rho} + O(nd)$  and query time  $n^\rho + dn^{o(1)}$ , where*

$$\rho \leq \frac{1}{2c^2 - 1} + o(1).$$

This is much better than the best LSH-based data structure, which has  $\rho = \frac{1}{c^2} + o(1)$ . For instance, for  $c = 2$ , the above theorem improves the query time from  $n^{1/4+o(1)}$  to  $n^{1/7+o(1)}$ , while using less memory.

Next, we describe the new approach at a high level.

## 4.2 Simplification of the problem

Before describing new techniques, it will be convenient to introduce a few simplifications. First, we can assume that  $d = \log^{1+o(1)} n$ , by applying Lemma 2.1. Second, we can reduce the general ANN problem over  $(\mathbb{R}^d, \ell_2)$  to the *spherical* case: where dataset and queries lie on the unit sphere  $S^{d-1} \subset \mathbb{R}^d$  (see [Raz17], pages 55–56). Both the dimension reduction and the reduction to the spherical case incur a negligible loss in the approximation<sup>10</sup>. After the reduction to the spherical case, the distance to the near neighbor  $r$  can be made to be any function of the number of points  $n$  that tends to zero as  $n \rightarrow \infty$  (for example,  $r = \frac{1}{\log \log n}$ ).

## 4.3 Data-independent partitions for a sphere

In light of the above discussion, we need to solve the  $(c, r)$ -ANN problem for  $S^{d-1}$ , where  $d = \log^{1+o(1)} n$  and  $r = o(1)$ . Even though the final data structure is based on data-dependent partitions, we start with developing a *data-independent* LSH scheme for the unit sphere, which will be later used as a building block.

The LSH scheme is parametrized by a number  $\eta > 0$ . Consider a sequence of i.i.d. samples from a standard  $d$ -dimensional Gaussian distribution  $N(0, 1)^d$ :  $g_1, g_2, \dots, g_t, \dots \in \mathbb{R}^d$ . The hash function  $h(x)$  of the point  $x \in S^{d-1}$  is then defined as  $\min_t \{t \geq 1 \mid \langle x, g_t \rangle \geq \eta\}$ . This LSH family gives the following exponent  $\rho$  for distances  $r$  and  $cr$ :

$$\rho = \frac{\log 1/p_1}{\log 1/p_2} = \frac{4 - c^2 r^2}{4 - r^2} \cdot \frac{1}{c^2} + \delta(r, c, \eta), \quad (1)$$

where  $\delta(r, c, \eta) > 0$  and  $\delta(r, c, \eta) \rightarrow 0$  as  $\eta \rightarrow \infty$ . Thus, the larger the value of the threshold  $\eta$  is, the more efficient the resulting LSH scheme is. At the same time,  $\eta$  affects the efficiency of hash functions. Indeed, one can show that with very high probability  $\max_{x \in S^{d-1}} h(x) \leq e^{(1+o(1))\eta^2/2} \cdot d^{O(1)}$ , which bounds the hashing time as well as the number of Gaussian vectors to store.

Consider the expression (1) for the exponent  $\rho$  in more detail. If  $r = o(1)$ , then we obtain  $\rho = \frac{1}{c^2} + o(1)$ , which matches the guarantee of the best data-independent LSH for  $\ell_2$ . This is hardly surprising, since, as was mentioned above, the general ANN problem over  $\ell_2$  can be reduced to the  $(c, r)$ -ANN problem over the sphere for  $r = o(1)$ . If  $r \approx 2/c$ , then  $\rho$  is close to zero, and, indeed, the  $(c, 2/c)$ -ANN problem on the sphere is trivial (any point can serve as an answer to any valid query).

Between these two extremes, there is a point  $r \approx \frac{\sqrt{2}}{c}$  that is crucial for the subsequent discussion. Since the distance between a pair of random points on  $S^{d-1}$  is close to  $\sqrt{2}$  with high probability, the problem where  $r$  is *slightly* smaller than  $\frac{\sqrt{2}}{c}$  has the following interpretation: if one is guaranteed to have a data point within distance  $r$  from the query, find a data point that is a bit closer to the query than a typical point on the sphere. For  $r \approx \frac{\sqrt{2}}{c}$ , the equation (1) gives exponent  $\rho \approx \frac{1}{2c^2-1}$ , which is significantly smaller than the bound  $\frac{1}{c^2}$  one is getting for  $r = o(1)$ . Later, using a certain data-dependent partitioning procedure, we will be able to reduce the *general* ANN problem on the sphere to this intermediate case of  $r \approx \frac{\sqrt{2}}{c}$ , thus obtaining the ANN data structure with the exponent  $\rho = \frac{1}{2c^2-1} + o(1)$ . This significantly improves upon the best possible LSH for  $\ell_2$  from Section 2, which yields  $\rho = \frac{1}{c^2} + o(1)$ .

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<sup>10</sup> Approximation  $c$  reduces to approximation  $c - o(1)$ .

#### 4.4 Data-dependent partitions

We now describe at a high level how to obtain a data structure with space  $n^{1+\rho}$  and query time  $n^\rho$ , where  $\rho = \frac{1}{2c^2-1} + o(1)$ , for the  $(c, r)$ -ANN problem on the sphere for general  $r > 0$ . If  $r \geq \frac{\sqrt{2}}{c} - o(1)$ , then we can simply use the data-independent LSH described above. Now suppose  $r$  is nontrivially smaller than  $\frac{\sqrt{2}}{c}$ .

We start with finding and removing *dense low-diameter clusters*. More precisely, we repeatedly find a point  $u \in S^{d-1}$  such that  $|P \cap B(u, \sqrt{2} - \varepsilon)| \geq \tau n$ , where  $\varepsilon, \tau = o(1)$ , and set  $P := P \setminus B(u, \sqrt{2} - \varepsilon)$ . We stop when there are no more dense clusters remaining. Then we proceed with clusters and the remainder separately. Each cluster is enclosed in a ball of radius  $1 - \Omega(\varepsilon^2)$  and processed recursively. For the remainder, we sample one partition from the data-independent LSH family described above, apply it to the dataset, and process each resulting part of the dataset recursively. During the query stage, we (recursively) query the data structure for *every* cluster (note that the number of clusters is at most  $1/\tau$ ), and for the remainder we query (again, recursively) a part of the partition, where the query belongs to. Each step of the aforementioned procedure makes progress as follows. For clusters, we decrease the radius by a factor of  $1 - \Omega(\varepsilon^2)$ . It means that we come slightly closer to the ideal case of  $r \approx \frac{\sqrt{2}}{c}$ , and the instance corresponding to the cluster becomes easier. For the remainder, we use the fact that there are at most  $\tau n$  data points closer than  $\sqrt{2} - \varepsilon$  to the query. Thus, when we apply the data-independent LSH, the expected number of data points in the same part as the query is at most  $(\tau + p_2)n$ , where  $p_2$  is the probability of collision under the LSH family for points at the distance  $\sqrt{2} - \varepsilon$ . We set  $\tau \ll p_2$ , thus the number of colliding data points is around  $p_2 n$ . At the same time, the probability of collision with the near neighbor is at least  $p_1$ , where  $p_1$  corresponds to the distance  $r$ . Since  $r < \frac{\sqrt{2}}{c}$ , we obtain an effective exponent of at most  $\frac{1}{2c^2-1} + o(1)$ . Note that we need to keep extracting the clusters recursively to be able to apply the above reasoning about the remainder set in each step.

One omission in the above high-level description is that the clusters are contained in smaller *balls* rather than *spheres*. This is handled by partitioning balls into thin annuli and treating them as spheres (introducing negligible distortion).

#### 4.5 Time–space trade-off

In [ALRW17], Theorem 4.1 has been extended to provide a smooth time–space trade-off for the ANN problem. Namely, it allows to decrease the query time at a cost of increasing the space and vice versa.

**Theorem 4.2.** *For every  $c > 1$  and every  $\rho_s, \rho_q$  such that*

$$c^2 \sqrt{\rho_q} + (c^2 - 1) \sqrt{\rho_s} \geq \sqrt{2c^2 - 1}, \quad (2)$$

*there exists a data structure for  $(c, r)$ -ANN over  $(\mathbb{R}^d, \ell_2)$  with space  $n^{1+\rho_s+o(1)} + O(nd)$  and query time  $n^{\rho_q+o(1)} + dn^{o(1)}$ .*

The bound (2) interpolates between:

- The near-linear space regime:  $\rho_s = 0$ ,  $\rho_q = \frac{2}{c^2} - \frac{1}{c^4}$ ;
- The “balanced” regime:  $\rho_s = \rho_q = \frac{1}{2c^2-1}$ , where it matches Theorem 4.1;
- The fast queries regime:  $\rho_s = \left(\frac{c^2}{c^2-1}\right)^2$ ,  $\rho_q = 0$ .

For example, for  $c = 2$ , one can obtain any of the following trade-offs: space  $n^{1+o(1)}$  and query time  $n^{7/16+o(1)}$ , space  $n^{8/7+o(1)}$  and query time  $n^{1/7+o(1)}$ , and space  $n^{16/9+o(1)}$  and query time  $n^{o(1)}$ .

Theorem 4.2 significantly improves upon the previous ANN data structures in various regimes [IM98, KOR00, Ind00b, Pan06, Kap15]. For example, it improves the dependence on  $\varepsilon$  in Theorem 2.2 from  $O(\log(1/\varepsilon)/\varepsilon^2)$  to  $O(1/\varepsilon^2)$ .

## 4.6 Impossibility results

Similarly to the data-independent case, it is natural to ask whether exponent  $\rho = \frac{1}{2c^2-1} + o(1)$  from Theorem 4.1 is optimal for data-dependent space partitions. In [AR16], it was shown that the above  $\rho$  is near-optimal in a properly formalized framework of data-dependent space partitions. This impossibility result can be seen as an extension of the results discussed in Section 2.4.

Specifically, [AR16] show that  $\rho \geq \frac{1}{2c^2-1}$ , where  $\rho = \frac{\log 1/p_1}{\log 1/p_2}$  for  $p_1$  and  $p_2$  being certain natural counterparts of the LSH collision probabilities for the data-dependent case, even when we allow the distribution on the partitions to depend on a dataset. This result holds under two further conditions. First, as in Section 2.4, we need to assume that  $p_2$  is not too small.

The second condition is specific to the data-dependent case, necessary to address another necessary aspect of the space partition. For any dataset, where all the points are sufficiently well separated, we can build an “ideal” space partition, with  $\rho = 0$ , simply by considering its Voronoi diagram. However, this is obviously not a satisfactory space partition: it is algorithmically hard to compute fast where in the partition a fixed query point  $q$  falls to — in fact, it is precisely equivalent to the original nearest neighbor problem! Hence, to be able to prove a meaningful lower bound on  $\rho$ , we would need to restrict the space partitions to have low run-time complexity (e.g., for a given point  $q$ , we can compute the part where  $q$  lies in, in time  $n^{o(1)}$ ). This precise restriction is well beyond reach of the current techniques (it would require proving computational lower bounds). Instead, [AR16] use a different, proxy restriction: they require that the *description complexity* of partitions is  $n^{1-\Omega(1)}$ . The latter restriction is equivalent to saying that the distribution of partitions (which may depend on the given dataset) is supported on a fixed (universal) family of partitions of the size  $2^{n^{1-\Omega(1)}}$ . This restriction, for instance, rules out the Voronoi diagram, since the latter has a description complexity of  $\Omega(n)$ . Furthermore, the description complexity of a randomized partition is a good proxy for the run-time complexity of a partition because in all the known constructions of random space partitions with a near-optimal  $\rho$ , the run-time complexity is at least the description complexity, which makes the requirement meaningful.

Overall, under the above two conditions, [AR16] show that  $\rho \geq \frac{1}{2c^2-1} - o(1)$  for data-dependent random space partitions, and hence Theorem 4.1 is essentially optimal in this framework.

## 4.7 ANN for $\ell_\infty$

In this subsection we will describe another type of data-dependent data structure, for the  $\ell_\infty$  norm. Historically, this was the first example of a data-dependent partitioning procedure used for ANN over high-dimensional spaces.

**Theorem 4.3** ([Ind01]). *For every  $0 < \varepsilon < 1$ , there exists a deterministic data structure for  $(c, 1)$ -ANN for  $(\mathbb{R}^d, \ell_\infty)$  with approximation  $c = O\left(\frac{\log \log d}{\varepsilon}\right)$ , space  $O(dn^{1+\varepsilon})$  and query time  $O(d \log n)$ .*

The algorithm relies on the following structural lemma.

**Lemma 4.4.** *Let  $P \subset \mathbb{R}^d$  be a set of  $n$  points and  $0 < \varepsilon < 1$ . Then:*

1. *Either there exists an  $\ell_\infty$ -ball of radius  $O\left(\frac{\log \log d}{\varepsilon}\right)$  that contains  $\Omega(n)$  points from  $P$ , or*

2. There exists a “good” coordinate  $i \in \{1, 2, \dots, d\}$  and a threshold  $u \in \mathbb{R}$  such that for the sets  $A = \{p \in P \mid p_i < u - 1\}$ ,  $B = \{p \in P \mid u - 1 \leq p_i \leq u + 1\}$  and  $C = \{p \in P \mid p_i > u + 1\}$  one has:

$$\left(\frac{|A| + |B|}{n}\right)^{1+\varepsilon} + \left(\frac{|B| + |C|}{n}\right)^{1+\varepsilon} \leq 1 \quad (3)$$

and  $|A|/n, |C|/n \geq \Omega(1/d)$ .

Using this lemma, we can build the data structure for  $(c, 1)$ -ANN for  $(\mathbb{R}^d, \ell_\infty)$  recursively. If there exists a ball  $B(x, R)$  with  $R = O\left(\frac{\log \log d}{\varepsilon}\right)$  such that  $|P \cap B(x, R)| \geq \Omega(n)$  (Case 1), then we store  $x$  and  $R$  and continue partitioning  $P \setminus B(x, R)$  recursively. If there exists a good coordinate  $i \in \{1, 2, \dots, d\}$  and a threshold  $u \in \mathbb{R}$  (Case 2), then we define sets  $A, B, C$  as in the above lemma and partition  $A \cup B$  and  $B \cup C$  recursively. We stop as soon as we reach a set that consists of  $O(1)$  points.

The query procedure works as follows. Suppose there is a point in  $P$  within distance 1 from  $q$  (“the near neighbor”). If we are in Case 1, we check if the query point  $q$  lies in  $B(x, R + 1)$ . If it does, we return any data point from  $B(x, R)$ ; if not, we query the remainder recursively. On the other hand, if we are in Case 2, we query  $A \cup B$  if  $q_i \leq u$ , and  $B \cup C$  otherwise. In this case we recurse on the part which is guaranteed to contain a near neighbor.

Overall, we always return a point within distance  $O\left(\frac{\log \log d}{\varepsilon}\right)$ , and it is straightforward to bound the query time by bounding the depth of the tree. We obtain the space bound of  $O(dn^{1+\varepsilon})$  by using the property (3) to bound the number of times points that are replicated in the Case 2 nodes.

Surprisingly, the approximation  $O(\log \log d)$  turns out to be *optimal* in certain restricted models of computation [ACP08, KP12], including for the approach from [Ind01].

## 5 Closest pair

A problem closely related to ANN is the closest pair problem, which can be seen as an “offline” version of ANN. Here, we are given a set  $P$  of  $n$  points, and we need to find a pair  $p, q \in P$  of distinct points that minimize their distance.

A trivial solution is to compute the distance between all possible  $\binom{n}{2}$  pairs of points and take the one that minimizes the distance. However this procedure has quadratic running time. As for the nearest neighbor problem, there is evidence that for, say,  $d$ -dimensional  $\ell_2$  space, the closest pair problem cannot be solved in time  $n^{2-\alpha}d^{O(1)}$  for any constant  $\alpha > 0$ .

As with  $c$ -ANN, we focus on the approximate version of the problem. Furthermore, we consider the *decision version*, where we need to find a pair of points that are below a certain threshold  $r$ . The formal definition (for the randomized variant) follows.

**Definition 5.1** ( $(c, r)$ -approximate close pair problem, or  $(c, r)$ -CP). *Given a set of points  $P \subset X$  of size  $n$ , if there exist distinct points  $p^*, q^* \in X$  with  $D(p^*, q^*) \leq r$ , find a pair of distinct points  $p, q \in P$  such that  $D(p, q) \leq cr$ , with probability at least  $2/3$ .*

The  $(c, r)$ -CP problem is closely related to the  $(c, r)$ -ANN problem because we can solve the former using a data structure for the latter. In particular, one can run the following procedure: partition  $P$  into two sets  $A, B$  randomly; build  $(c, r)$ -ANN on the set  $A$ ; query every point  $q \in B$ . It is easy to see that one such run succeeds in solving a  $(c, r)$ -approximate close pair with probability at least  $1/2 \cdot 2/3$ . Repeating the procedure 3 times is enough to guarantee a success probability of  $2/3$ . If  $(c, r)$ -ANN under the desired metric can be solved with query time  $Q(n)$  and preprocessing time  $S(n)$ , we obtain a solution for  $(c, r)$ -CP running in time  $O(S(n) + nQ(n))$ . For example,



applying the reduction from above for  $(\mathbb{R}^d, \ell_p)$  space for  $p \in \{1, 2\}$ , we immediately obtain an algorithm running in  $O(dn^{1+\rho})$  time, where  $\rho = \frac{1}{2c^p-1} + o(1)$  (Section 4).

Focusing on the case of  $\ell_2$ , and approximation  $c = 1 + \varepsilon$ , the above algorithm has runtime  $O(n^{2-4\varepsilon+O(\varepsilon^2)}d)$ . It turns out that, for the  $\ell_2$  norm, one can obtain algorithms with a better dependence on  $\varepsilon$ , for small  $\varepsilon$ . In particular, the line of work from [Val15, KKK16, ACW16] led to the following algorithm:

**Theorem 5.2** ([ACW16]). *Fix dimension  $d \geq 1$ ,  $r > 0$ , and  $\varepsilon \in (0, 1/2)$ . Then, for any set of  $n$  points in  $\mathbb{R}^d$ , one can solve the  $(1 + \varepsilon, r)$ -CP over  $\ell_2$  in time  $O(n^{2-\Omega(\varepsilon^{1/3}/\log(1/\varepsilon))} + dn)$ , with constant probability.*

Note that the running time bound in the above theorem is better than that obtained using LSH data structures, for small enough  $\varepsilon$ .

The main new technical ingredient is the *fast matrix multiplication* algorithm. In particular, suppose we want to multiply two matrices of size  $n \times m$  and  $m \times n$ . Doing so naïvely takes time  $O(n^2m)$ . Starting with the work of [Str69], there has been substantial work to improve this runtime; see also [Wil12]. Below we state the running time of a fast matrix multiplication algorithm due to [Cop82], which is most relevant for this section.

**Theorem 5.3** ([Cop82]). *Fix  $n \geq 1$  and let  $m \geq 1$  be such that  $m \leq n^{0.172}$ . One can compute the product of two matrices of sizes  $n \times m$  and  $m \times n$  in  $O(n^2 \log^2 n)$  time.*

## 5.1 Closest pair via matrix multiplication

We now sketch the algorithm for the closest pair from [Val15], which obtains  $O(n^{2-\Omega(\sqrt{\varepsilon})}d)$  time. The algorithm is best described in terms of *inner products*, as opposed to distances as before. In particular, suppose we have a set of points  $P \subset \mathcal{S}^d$  of unit norm, where all pairs of points have inner product in the range  $[-\theta, \theta]$ , except for one “special” pair that has inner product at least  $c\theta$ , for some scale  $\theta > 0$  and approximation  $c = 1 + \varepsilon$ . Now the problem is to find this special pair—we term this problem  $(c, \theta)$ -IP problem. We note that we can reduce  $(1 + \varepsilon, r)$ -CP over  $\ell_2$  to  $(1 + \Omega(\varepsilon), 1/2)$ -IP, by using the embedding of [Sch42], or Lemma 2.3 of [KOR00].

A natural approach to the IP problem is to multiply two  $n \times d$  matrices: if we consider the matrix  $M$  where the rows are the points of  $P$ , then  $MM^t$  will have a large off-diagonal entry precisely for the special pair of points. This approach however requires at least  $n^2$  computation time, since even the output of  $MM^t$  has size  $n^2$ . Nevertheless, an extension of this approach gives a better run-time when  $c$  is very large (and hence  $\theta < 1/c$  very small, i.e., all points except for the special pair are near-orthogonal). In particular, partition randomly the vectors from  $P$  into  $n/g$  groups  $S_1, \dots, S_{n/g}$ , each of size  $O(g)$ . For each group  $i$ , we sum the vectors  $S_i$  with random signs, obtaining vectors  $v_i = \sum_{p_j \in S_i} \chi_j p_j$ , where  $p_j$  are the points in  $P$  and  $\chi_j$  are Rademacher random variables. Now the algorithm forms a matrix  $M$  with  $v_i$ ’s as rows, and computes  $MM^t$  using fast matrix multiplication (Theorem 5.3). The two special points are separated with probability  $1 - g/n$ . Conditioning on this event, without loss of generality, we can assume that they are in group 1 and 2 respectively. Then, it is easy to note that  $|(MM^t)_{12}| \approx \Theta(c \cdot \theta)$ , whereas, for  $(i, j) \neq (1, 2)$  and  $i \neq j$ , we have that  $|(MM^t)_{ij}| \approx O(g \cdot \theta)$  with constant probability. Hence, we can identify the special pair in the product  $MM^t$  as long as  $c \gg g$ , and yields runtime  $O(n^2/g^2)$ , i.e., a  $g^2 \ll c^2$  speed-up over the naïve algorithm (note that Theorem 5.3 requires that  $d < n^{0.172}$ ).

The above approach requires  $c$  to be very large, and hence the challenge is whether we can reduce the case of  $c = 1 + \varepsilon$  to the case of large  $c$ . Indeed, one method is to use tensoring: for a fixed parameter  $k$  and any two vectors  $x, y \in \mathbb{R}^d$ , we consider  $x^{\otimes k}, y^{\otimes k} \in \mathbb{R}^{d^k}$ , for which

$\langle x^{\otimes k}, y^{\otimes k} \rangle = (\langle x, y \rangle)^k$ . Thus tensoring reduces the problem of  $(1 + \varepsilon, 1/2)$ -IP to  $((1 + \varepsilon)^k, 2^{-k})$ -IP, and hence we hope to use the above algorithm for  $c = (1 + \varepsilon)^k \approx e^{\varepsilon k}$ . If we use  $t = \zeta \ln n$ , for small constant  $\zeta$ , we obtain  $c = n^{\varepsilon \zeta}$ , and hence we obtain a speed-up of  $g^2 \approx c^2 = n^{2\varepsilon \zeta}$ . One caveat here is that, after tensoring the vectors, we obtain vectors of dimension  $d^k$ , which could be much larger than  $n$ —then even writing down such vectors would take  $\Omega(n^2)$  time. Yet, one can use a dimension reduction method, like Lemma 2.1, to reduce dimension to  $O(\frac{\log n}{\theta^k}) = \tilde{O}(n^{\zeta \ln 2})$ , which is enough to preserve all inner products up to additive, say,  $0.1 \cdot \theta^k$ . There are further details (e.g., we cannot afford to get high-dimensional vectors in the first place, even if we perform dimension-reduction), see [Val15, KKK16] for more details.

The above algorithm yields a speed-up of the order of  $n^{O(\varepsilon)}$ , i.e., comparable to the speed-up via the LSH methods. To obtain a better speed-up, like in the Theorem 5.2, one can replace the tensoring transformation with a more efficient one. Indeed, one can employ an *asymmetric* embedding  $f, g : \mathbb{R}^d \rightarrow \mathbb{R}^m$ , with the property that for any unit-norm vectors  $x, y$ , we have that  $\langle f(x), g(y) \rangle = p(\langle x, y \rangle)$ , where  $p(\cdot)$  is a polynomial of choice. In particular, we require a polynomial  $p(\cdot)$  that is small on the interval  $[-\theta, \theta]$ , as large as possible on  $[(1 + \varepsilon)\theta, 1]$ , and  $p(1)$  is bounded. Note that the tensoring operation implements such an embedding with  $p(a) = a^k$  and where  $f(x) = g(x) = x^{\otimes k}$ . However, there are more efficient polynomials: in fact, the optimal such polynomial is the Chebyshev polynomial. For example, for the degree- $k$  Chebyshev polynomial  $T_k(\cdot)$ , we have that  $T_k(1 + \varepsilon)/T_k(1) \approx e^{\sqrt{\varepsilon}k}$ , which is in contrast to the above polynomial  $p(a) = a^k$ , for which  $p(1 + \varepsilon)/p(1) \approx e^{\varepsilon k}$ .

Using the Chebyshev polynomials, one can obtain a runtime of  $n^{2-\Omega(\sqrt{\varepsilon})}$  for the IP and hence CP problem. To obtain the improved result from Theorem 5.2, [ACW16] employ *randomized* polynomials, i.e., a distribution over polynomials where  $p(\cdot)$  is small/large only with a certain probability. Without going into further details, the theorem below states the existence of such polynomials, which are used to obtain  $n^{2-\Omega(\varepsilon^{1/3}/\log(1/\varepsilon))}$  run-time for the  $(1 + \varepsilon, r)$ -CP problem.

**Theorem 5.4** ([ACW16]). *Fix  $d \geq 1$ ,  $\theta \geq 1$ ,  $s \geq 1$ , and  $\varepsilon > 0$ . There exists a distribution over polynomials  $P : \{0, 1\}^d \rightarrow \mathbb{R}$  of degree  $O(\varepsilon^{-1/3} \log s)$ , such that we have the following for any  $x \in \{0, 1\}^d$ :*

- *if  $\sum_{i=1}^d x_i \leq \theta$ , then  $|P(x)| \leq 1$  with probability at least  $1 - 1/s$ ;*
- *if  $\sum_{i=1}^d x_i \in (\theta, (1 + \varepsilon)\theta)$ , then  $|P(x)| > 1$  with probability at least  $1 - 1/s$ ;*
- *if  $\sum_{i=1}^d x_i > (1 + \varepsilon)\theta$ , then  $|P(x)| \geq s$  with probability at least  $1 - 1/s$ .*

## 6 Extensions

In this section, we discuss several techniques that significantly extend the class of spaces which admit efficient ANN data structures.

### 6.1 Metric embeddings

So far, we have studied the ANN problem over the  $\ell_1$ ,  $\ell_2$  and  $\ell_\infty$  distances. A useful approach is to *embed* a metric of interest into  $\ell_1/\ell_2/\ell_\infty$  and use one of the data structures developed for the latter spaces.

### 6.1.1 Deterministic embeddings

**Definition 6.1.** For metric spaces  $\mathcal{M} = (X, D_X)$ ,  $\mathcal{N} = (Y, D_Y)$  and for  $D \geq 1$ , we say that a map  $f: X \rightarrow Y$  is a bi-Lipschitz embedding with distortion  $D$  if there exists  $\lambda > 0$  such that for every  $x_1, x_2 \in X$  one has:

$$\lambda D_X(x_1, x_2) \leq D_Y(f(x_1), f(x_2)) \leq D \cdot \lambda D_X(x_1, x_2).$$

A bi-Lipschitz embedding of  $\mathcal{M}$  into  $\mathcal{N}$  with distortion  $D$  together with a data structure for  $(c, r)$ -ANN over  $\mathcal{N}$  immediately implies a data structure for  $(cD, r')$ -ANN over  $\mathcal{M}$ , where  $r' = \frac{r}{\lambda D}$ . However, space and query time of the resulting data structure depend crucially on the *computational efficiency* of the embedding, since, in particular, the query procedure requires evaluating the embedding on a query point.

As the following classic results show, any finite-dimensional normed or finite metric space can be embedded into finite-dimensional  $\ell_\infty$  with small distortion.

**Theorem 6.2** (Fréchet–Kuratowski, [Fré06, Kur35]). *If  $\mathcal{M}$  is a finite metric space, which consists of  $N$  points, then  $\mathcal{M}$  embeds into  $(\mathbb{R}^N, \ell_\infty)$  with distortion  $D = 1$  (isometrically).*

**Theorem 6.3** (see, e.g., [Woj96]). *For every  $\varepsilon > 0$ , every normed space  $(\mathbb{R}^d, \|\cdot\|)$  embeds with distortion  $1 + \varepsilon$  into  $(\mathbb{R}^{d'}, \ell_\infty)$ , where  $d' = O(1/\varepsilon)^d$ , via a linear map.*

However, the utility of Theorems 6.2 and 6.3 in the context of the ANN problem is limited, since the required dimension of the target  $\ell_\infty$  space is very high (in particular, Theorem 6.3 gives a data structure with *exponential* dependence on the dimension). Moreover, even if we allow the distortion  $D$  of an embedding to be a large constant, the target dimension can not be improved much. As has been shown in [Mat97], one needs at least  $N^{\Omega(1/D)}$ -dimensional  $\ell_\infty$  to “host” all the  $N$ -point metrics with distortion  $D$ . For  $d$ -dimensional norms, even as simple as  $\ell_2$ , the required dimension is  $2^{\Omega_D(d)}$  [FLM77, Bal97].

More generally, (lower-dimensional)  $\ell_\infty$  turns out to be not so useful of a target space, and only a handful of efficient embeddings into  $\ell_\infty$  are known (for instance, such an embedding has been constructed in [FCI99] for the Hausdorff distance). Luckily, the situation drastically improves, if we allow *randomized* embeddings, see Section 6.1.2 for the examples.

Instead of  $\ell_\infty$ , one can try to embed a metric of interest into  $\ell_1$  or  $\ell_2$ . Let us list a few cases, where such embeddings lead to efficient ANN data structures.

- Using the result from [JS82], one can embed  $(\mathbb{R}^d, \ell_p)$  for  $1 < p \leq 2$  into  $(\mathbb{R}^{d'}, \ell_1)$  with distortion  $1 + \varepsilon$ , where  $d' = O(d/\varepsilon^2)$ . Moreover, the corresponding map is linear and hence efficient to store and apply. This reduction shows that the ANN problem over  $\ell_p$  for  $1 < p \leq 2$  is no harder than for the  $\ell_1$  case. However, later in this section we will show how to get a better ANN algorithm for the  $\ell_p$  case using a different embedding.
- For the Wasserstein-1 distance (a.k.a. the Earth-Mover distance in the computer science literature) between probability measures defined on  $\{1, 2, \dots, d\}^k$ , one can use the results from [Cha02, IT03, NS07], to embed it into  $(\mathbb{R}^{d^{O(k)}}, \ell_1)$  with distortion  $O(k \log d)$ .
- The Levenshtein distance (a.k.a. edit distance) over the binary strings  $\{0, 1\}^d$  can be embedded into  $(\mathbb{R}^{d^{O(1)}}, \ell_1)$  with distortion  $2^{O(\sqrt{\log d \log \log d})}$  [OR07].

Let us note that there exist generic results concerned with embeddings into  $\ell_1/\ell_2$  similar to Theorem 6.2 and Theorem 6.3.

**Theorem 6.4** ([Bou85, LLR95]). *Any  $N$ -point metric embeds into  $(\mathbb{R}^{O(\log N)}, \ell_2)$  with distortion  $O(\log N)$ .*

**Theorem 6.5** ([Joh48, Bal97]). *Any normed space  $(\mathbb{R}^d, \|\cdot\|)$  embeds into  $(\mathbb{R}^d, \ell_2)$  with distortion  $\sqrt{d}$  via a linear map.*

Theorem 6.4 does not give an embedding efficient enough for the ANN applications: computing it in one point requires time  $\Omega(N)$ . At the same time, Theorem 6.5 is efficient and, together with  $\ell_2$  data structures, gives an ANN data structure for a general  $d$ -dimensional norm with approximation  $O(\sqrt{d})$ .

Since the ANN problem is defined for two specific distance scales ( $r$  and  $cr$ ), we do not need the full power of bi-Lipschitz embeddings and sometimes can get away with weaker notions of embeddability. For example, the following theorem follows from the results of [Sch37].

In the theorem,  $\ell_2(\mathbb{N})$  denotes the space of infinite sequences  $(a_i)_{i=1}^\infty$  such that  $\sum_i |a_i|^2 < +\infty$  and the norm of the sequence  $\|a\|_2$  is equal to  $(\sum_i |a_i|^2)^{1/2}$ .

**Theorem 6.6.** *For every  $1 \leq p < 2$  and every  $d \geq 1$ , there exists a map  $f: \mathbb{R}^d \rightarrow \ell_2(\mathbb{N})$  such that for every  $x, y \in \mathbb{R}^d$ , one has:*

$$\|f(x) - f(y)\|_2^2 = \|x - y\|_p^p.$$

This embedding allows to use an ANN data structure for  $\ell_2$  with approximation  $c$  to get an ANN data structure for  $\ell_p$  with approximation  $c^{2/p}$ . However, for this we need to make the embedding computationally efficient. In particular, the target must be finite-dimensional. This can be done, see [Ngu14] for details. As a result, for the  $\ell_p$  distance for  $1 \leq p < 2$ , we are able to get the result similar to the one given by Theorem 4.2, where in (2)  $c^2$  is replaced with  $c^p$  everywhere.

### 6.1.2 Randomized embeddings

It would be highly desirable to utilize the fact that every metric embeds well into  $\ell_\infty$  (Theorems 6.2 and 6.3) together with the ANN data structure for  $\ell_\infty$  from Section 4.7. However, as discussed above, spaces as simple as  $(\mathbb{R}^d, \ell_1)$  or  $(\mathbb{R}^d, \ell_2)$  require the target  $\ell_\infty$  to have  $2^{\Omega(d)}$  dimensions to be embedded with small distortion. It turns out, this can be remedied by allowing embeddings to be *randomized*. In what follows, we will consider the case of  $(\mathbb{R}^d, \ell_1)$ , and then generalize the construction to other metrics.

The randomized embedding of  $(\mathbb{R}^d, \ell_1)$  into  $(\mathbb{R}^d, \ell_\infty)$  is defined as follows: we generate  $d$  i.i.d. samples  $u_1, u_2, \dots, u_d$  from the exponential distribution with parameter 1, and then the embedding  $f$  maps a vector  $x \in \mathbb{R}^d$  into

$$\left( \frac{x_1}{u_1}, \frac{x_2}{u_2}, \dots, \frac{x_d}{u_d} \right).$$

Thus, the resulting embedding is linear. Besides that, it is extremely efficient to store ( $d$  numbers) and apply ( $O(d)$  time).

Let us now understand how  $\|f(x)\|_\infty$  is related to  $\|x\|_1$ . The analysis uses (implicitly) the *min-stability* property of the exponential distribution. One has for every  $t > 0$ :

$$\Pr_f[\|f(x)\|_\infty \leq t] = \prod_{i=1}^d \Pr \left[ \frac{|x_i|}{u_i} \leq t \right] = \prod_{i=1}^d \Pr \left[ u_i \geq \frac{|x_i|}{t} \right] = \prod_{i=1}^d e^{-|x_i|/t} = e^{-\|x\|_1/t}.$$

The random variable  $\|f(x)\|_\infty$  does not have a finite first moment, however its mode is in the point  $t = \|x\|_1$ , which allows us to use  $\|f(x)\|_\infty$  to estimate  $\|x\|_1$ . It is immediate to show that for

every  $\delta > 0$ , there exist  $C_1, C_2 > 1$  with  $C_1 = O(\log(1/\delta))$  and  $C_2 = O(1/\delta)$  such that for every  $x$ , one has:

$$\Pr_f \left[ \|f(x)\|_\infty \geq \frac{\|x\|_1}{C_1} \right] \geq 1 - \delta \quad (4)$$

and

$$\Pr_f [\|f(x)\|_\infty \leq C_2 \cdot \|x\|_1] \geq 1 - \delta \quad (5)$$

Thus, the map  $f$  has distortion  $O\left(\frac{\log(1/\delta)}{\delta}\right)$  with probability  $1 - \delta$ . However, unlike the deterministic case, the randomized guarantees (4) and (5) are not sufficient for the reduction between ANN data structures (if  $\delta \gg 1/n$ ). This is because the lower bound on  $\|f(x)\|_\infty$  must apply simultaneously to all “far” points. In order to obtain a desired reduction, we need to use slightly different parameters. Specifically, for  $0 < \varepsilon < 1$  one has:

$$\Pr_f \left[ \|f(x)\|_\infty \geq \Omega\left(\frac{\|x\|_1}{\log n}\right) \right] \geq 1 - \frac{1}{10n}$$

and

$$\Pr_f \left[ \|f(x)\|_\infty \leq O\left(\frac{\|x\|_1}{\varepsilon \cdot \log n}\right) \right] \geq n^{-\varepsilon}.$$

This allows us to reduce the  $(c/\varepsilon, r)$ -ANN problem over  $(\mathbb{R}^d, \ell_1)$  to  $n^{O(\varepsilon)}$  instances of the  $(c, r')$ -ANN problem over  $(\mathbb{R}^d, \ell_\infty)$ . Indeed, we sample  $n^{O(\varepsilon)}$  i.i.d. maps  $f_i$  as described above and solve the ANN problem over  $\ell_\infty$  on the image of  $f_i$ . Far points remain being far with probability  $1 - 1/10n$  each. Using the linearity of expectation and the Markov inequality, we observe that, with probability at least 0.9, no far point come close enough to the query point. At the same time, with probability at least  $n^{-\varepsilon}$ , the near neighbor does not move too far away, so, with high probability, at least one of the  $n^{O(\varepsilon)}$  data structures succeeds. This reduction is quite similar to the use of Locality-Sensitive Hashing in Section 2.2.

As a result, we get an ANN data structure for  $(\mathbb{R}^d, \ell_1)$  with approximation  $O\left(\frac{\log \log d}{\varepsilon^2}\right)$ , query time  $O(dn^\varepsilon)$  and space  $O(dn^{1+\varepsilon})$ . This is worse than the best ANN data structure for  $\ell_1$  based on (data-dependent) space partitions. However, the technique we used is very versatile and generalizes easily to many other distances. The  $\ell_1$  embedding was first used in [AIK09]. Later, it was generalized [And09] to  $\ell_p$  spaces for  $p \geq 1$ . To get such an embedding, one can divide every coordinate by the  $(1/p)$ -th power of an exponential random variable. Finally, in [ANN<sup>+</sup>17b] the same technique has been shown to work for Orlicz norms and top- $k$  norms, which we define next.

**Definition 6.7.** Let  $\psi: [0; +\infty) \rightarrow [0; +\infty)$  be a non-negative monotone increasing convex function with  $\psi(0) = 0$ . Then, an Orlicz norm  $\|\cdot\|_\psi$  over  $\mathbb{R}^d$  is given by its unit ball  $K_\psi$ , defined as follows:

$$K_\psi = \left\{ x \in \mathbb{R}^d \left| \sum_{i=1}^d \psi(|x_i|) \leq 1 \right. \right\}.$$

Clearly,  $\ell_p$  norm for  $p < \infty$  is Orlicz for  $\psi(t) = t^p$ .

**Definition 6.8.** For  $1 \leq k \leq d$ , we define the top- $k$  norm of a vector from  $\mathbb{R}^d$  as the sum of  $k$  largest absolute values of the coordinates.

The top-1 norm is simply  $\ell_\infty$ , while top- $d$  corresponds to  $\ell_1$ .

To embed an Orlicz norm  $\|\cdot\|_\psi$  into  $\ell_\infty$ , we divide the coordinates using a random variable  $X$  with the c.d.f.  $F_X(t) = \Pr[X \leq t] = 1 - e^{-\psi(t)}$ . To embed the top- $k$  norm, we use a truncated exponential distribution. All of the above embeddings introduce only a constant distortion.

Let us note that for the  $\ell_p$  norms one can achieve approximation  $2^{O(p)}$  [NR06, BG15], which is an improvement upon the above  $O(\log \log d)$  bound if  $p$  is sufficiently small.



## 6.2 ANN for direct sums

In this section we describe a vast generalization of the ANN data structure for  $\ell_\infty$  from Section 4.7. Namely, we will be able to handle *direct sums* of metric spaces.

**Definition 6.9.** Let  $M_1 = (X_1, D_1)$ ,  $M_2 = (X_2, D_2)$ ,  $\dots$ ,  $M_k = (X_k, D_k)$  be metric spaces and let  $\|\cdot\|$  be a norm over  $\mathbb{R}^k$ . Then the  $\|\cdot\|$ -direct sum of  $M_1, M_2, \dots, M_k$  denoted by  $\left(\bigoplus_{i=1}^k M_i\right)_{\|\cdot\|}$  is a metric space defined as follows. The ground set is the Cartesian product  $X_1 \times X_2 \times \dots \times X_k$ . The distance function  $D$  is given by the following formula.

$$D((x_1, x_2, \dots, x_k), (y_1, y_2, \dots, y_k)) = \|(D_1(x_1, y_1), D_2(x_2, y_2), \dots, D_k(x_k, y_k))\|.$$

It turns out that for many interesting norms  $\|\cdot\|$  the following holds. If for metrics  $M_1, M_2, \dots, M_k$  there exist efficient ANN data structures, then the same holds for  $\left(\bigoplus_{i=1}^k M_i\right)_{\|\cdot\|}$  (with a mild loss in the parameters).

The first result of this kind was shown in [Ind02]<sup>11</sup> for the case of  $\ell_\infty$ -direct sums. In what follows we denote by  $d$  the “complexity” of each metric  $M_i$ . That is, we assume it takes  $O(d)$  time to compute the distance between two points, and that a point requires  $O(d)$  space to store.

**Theorem 6.10.** Let  $c > 1$ ,  $r > 0$  and  $0 < \varepsilon < 1$ . Suppose that each  $M_i$  admits a  $(c, r)$ -ANN data structure for  $n$ -point sets with space  $n^{1+\rho}$  (in addition to storing the dataset) for some  $\rho \geq 0$  and query time  $Q(n)$ . Then, there exists a data structure for  $(c', r)$ -ANN over  $\left(\bigoplus_{i=1}^k M_i\right)_\infty$ , where  $c' = O\left(\frac{c \log \log n}{\varepsilon}\right)$ , the space is  $O(n^{1+\rho+\varepsilon})$  (in addition to storing the dataset), and the query time is  $Q(n) \cdot \log^{O(1)} n + O(dk \log n)$ .

Informally speaking, compared to data structures for  $M_i$ , the data structure for  $\left(\bigoplus_i M_i\right)_\infty$  loses  $\frac{\log \log n}{\varepsilon}$  in approximation,  $n^\varepsilon$  in space, and  $\log^{O(1)} n$  in query time.

Later, the result of [Ind02] was significantly extended [Ind04, AIK09, And09, ANN<sup>+</sup>17b], to support  $\|\cdot\|$ -direct sums where  $\|\cdot\|$  is an  $\ell_p$  norm, an Orlicz norm, or a top- $k$  norm. The main insight is that we can use the randomized embeddings of various norms into  $\ell_\infty$  developed in Section 6.1.2, to reduce the case of  $\|\cdot\|$ -direct sums to the case of  $\ell_\infty$ -direct sums. Indeed, we described how to reduce the ANN problem over several classes of norms to  $n^\varepsilon$  instances of ANN over the  $\ell_\infty$  distance at a cost of losing  $O(1/\varepsilon)$  in the approximation. It is not hard to see that the exact same approach can be used to reduce the ANN problem over  $\left(\bigoplus_{i=1}^k M_i\right)_{\|\cdot\|}$  to  $n^\varepsilon$  instances of ANN over  $\left(\bigoplus_{i=1}^k M_i\right)_\infty$  also at a cost of losing  $O(1/\varepsilon)$  in approximation.

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<sup>11</sup>In [Ind02], a slightly weaker version of Theorem 6.10 has been stated. First, it assumed *deterministic* data structures for the spaces  $M_i$ . This is straightforward to address by boosting the probability of success for data structures for  $M_i$  using repetition. Second, the resulting space bound [Ind02] was worse. An improvement to the space bound has been described in Appendix A of the arXiv version of [ANN<sup>+</sup>17b]. Finally, the paper [Ind02] assumes ANN data structures for  $M_i$  with a slightly stronger guarantee. Namely, each point is assigned a *priority* from 1 to  $n$ , and if the near neighbor has priority  $t$ , we must return a point with priority at most  $t$ . It is not hard to solve the version with priorities using a standard ANN data structure (with  $\log^{O(1)} n$  loss in space and query time). A naïve reduction builds an ANN data structure for points with priority at most  $t$  for every  $t$ . Then, we can run a binary search over the resulting priority. However, this gives a *linear in  $n$*  loss in space. To rectify this, we use a standard data structure technique: the decomposition of an interval into  $O(\log n)$  *dyadic intervals*, i.e., intervals of the form  $[2^k \cdot l + 1; 2^k \cdot (l + 1)]$  for integer  $k, l$ . Thus, we build an ANN data structure for every dyadic interval of priorities. This still gives  $O(n)$  ANN data structures, however, each data point participates in at most  $O(\log n)$  of them.

### 6.3 Embeddings into direct sums

As Section 6.2 shows, for a large class of norms  $\|\cdot\|$ , we can get an efficient ANN data structure for any  $\|\cdot\|$ -direct sum of metrics that admit efficient ANN data structures. This gives a natural approach to the ANN problem: embed a metric of interest into such a direct sum.

This approach has been successful in several settings. In [Ind02], the Fréchet distance between two sequences of points in a metric space is embedded into an  $\ell_\infty$ -direct sums of Fréchet distances between shorter sequences. Together with Theorem 6.10, this was used to obtain an ANN data structure for the Fréchet distance. In [AIK09], it is shown how to embed the Ulam metric (which is the edit distance between permutations of length  $d$ ) into  $\left(\bigoplus^d \left(\bigoplus^{O(\log d)} (\mathbb{R}^d, \ell_1)\right)\right)_{\ell_\infty}_{\ell_2^2}$  with a constant distortion which gives an ANN data structure with doubly-logarithmic approximation. At the same time, the Ulam distance requires distortion  $\Omega\left(\frac{\log d}{\log \log d}\right)$  to embed into  $\ell_1$  [AK10]. This shows that (lower-dimensional) direct sums form a strictly more “powerful” class of spaces than  $\ell_1$  or  $\ell_2$ . Finally, in [ANN<sup>+</sup>17b], it is shown that *any* symmetric norm over  $\mathbb{R}^d$  is embeddable into  $\left(\bigoplus_{i=1}^{d^{O(1)}} \left(\bigoplus_{j=1}^d X_{ij}\right)_1\right)_\infty$  with constant distortion, where  $X_{ij}$  is  $\mathbb{R}^d$  equipped with the top- $j$  norm. Together with the results from Section 6.1.2 and Section 6.2, this gives an ANN algorithm with approximation  $(\log \log n)^{O(1)}$  for general *symmetric*<sup>12</sup> norms.

### 6.4 ANN for general norms

For *general*  $d$ -dimensional norms, the best known ANN data structure is obtained by combining Theorem 6.5 with an efficient ANN data structure for  $\ell_2$  (for example, the one given by Theorem 4.1). This approach gives approximation  $O(\sqrt{d/\varepsilon})$  for space  $d^{O(1)} \cdot n^{1+\varepsilon}$  and query time  $d^{O(1)} \cdot n^\varepsilon$  for every constant  $0 < \varepsilon < 1$ . Very recently, the approximation  $O(\sqrt{d/\varepsilon})$  has been improved to  $O\left(\frac{\log d}{\varepsilon^2}\right)$  [ANN<sup>+</sup>17a] for the same space and time bounds if one is willing to relax the model of computation to the *cell-probe model*, where the query procedure is charged for *memory accesses*, but any computation is free. This ANN data structure heavily builds on a recent geometric result from [Nao17]: a bi-Lipschitz embedding (see Definition 6.1) of the shortest-path metric of *any*  $N$ -node expander graph [HLW06] into an *arbitrary*  $d$ -dimensional normed space must have distortion at least  $\Omega(\log_d N)$ . At a very high level, this non-embeddability result is used to claim that any large bounded-degree graph, which *does* embed into a normed space, can not be an expander, and hence it must have a sparse cut. The existence of the sparse cut is then used, via a duality argument, to build a (data-dependent) random space partition family for a general  $d$ -dimensional normed space. The latter family is used to obtain the final data structure.

This approach can be further extended for several norms of interest to obtain proper, *time-efficient* ANN data structures, with even better approximations. For instance, [ANN<sup>+</sup>17a] show how to get ANN with approximation  $O(p)$  for the  $\ell_p$  norms, improving upon the bound  $2^{O(p)}$  from [NR06, BG15]. Finally, for the Schatten- $p$  norms of matrices, defined as the  $\ell_p$  norm of the vector of singular values, one obtains approximation  $O(p)$  as well, while the previous best approximation was polynomial in the matrix size (by relating the Schatten- $p$  norm to the Frobenius norm).

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<sup>12</sup>Under permutations and negations of the coordinates.

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