Curse of Dimensionality in Pivot-based Indexes

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Abstract—We offer a theoretical validation of the curse of dimensionality in the pivot-based indexing of datasets for similarity search, by proving, in the framework of statistical learning, that in high dimensions no pivot-based indexing scheme can essentially outperform the linear scan.

A study of the asymptotic performance of pivot-based indexing schemes is performed on a sequence of datasets modeled as samples picked in i.i.d. fashion from a sequence of metric spaces. We allow the size of the dataset to grow in relation to dimension, such that the dimension is superlogarithmic but subpolynomial in the size of the dataset. The number of pivots is sublinear in the size of the dataset. We pick the least restrictive cost model of similarity search where we count each distance calculation as a single computation and disregard the rest.

We demonstrate that if the intrinsic dimension of the spaces in the sense of concentration of measure phenomenon is linear in dimension, then the performance of similarity search pivot-based indexes is asymptotically linear in the size of the dataset.

Keywords—Data structures; Similarity search; Curse of dimensionality; Concentration of Measure;

I. INTRODUCTION

The problem of similarity search in databases is addressed by building indexing schemes of various types [Cia97], [Cha01], [Cha05], [Zez05]. The goal of such structures is that a search algorithm can exploit them to perform similarity search in time sublinear in the database size. That indexing schemes do not scale well with increasing dimension has been referred to as “the curse of dimensionality” [Bey99], [Ind04].

We feel that in order to gain a better insight into the nature of the curse of dimensionality, it is necessary to have a precise mathematical understanding of the geometric and algorithmic aspects of what happens in genuinely high-dimensional datasets. With this purpose, we have chosen to analyse one of the most popular indexing schemes for similarity search, the one based on pivots [Bus03], [Cha01]. The mathematical setting for our analysis is a rigorous model of statistical learning theory [Bia89], [Dev97], [Vap98], [Vid05], where datasets are drawn randomly from domains of increasing dimension.

This probabilistic setting is similar to that used in a previous asymptotic analysis of similarity search [Sha06]. We also adopt a cost model where we count distance computations only, in line with [Sha06]. Unlike this previous work, we let both the dimension $d$ and the size of the dataset $n$ grow as described in [Ind04]. We also make the distinction between the dataset and the data space mathematically explicit. In particular we emphasize that statements of the type “all indexing scheme will degenerate to linear scan with increasing dimension” (to paraphrase [Web98]) will always need to be qualified with estimates of the probability. For it is not impossible to sample a hypercube uniformly and come up with a “distribution with a million clusters” [Sha06].

Our analysis is done on a sequence of datasets that exhibit the concentration of measure phenomenon [Gro83], [Mil86] (Sect. V), a concept linked to what is called in [Sha06] workloads with vanishing variance. It is also in terms of this concentration of measure that we define the dimension $d$. To show that the above situation with a million clusters cannot happen (too often) we study the convergence of empirical probabilities to their true values using a result from Statistical Learning Theory [Vap98]. We introduce a property of a sequence of spaces which is enough to invoke this result.

The conclusion of our analysis (Sect. VIII) is that for high dimensional datasets the class of pivot-based indexing schemes cannot significantly outperform the baseline linear scan of checking every element of the database.

II. METRICS, MEASURES, AND DATASETS

We model the dataset as a sample of a metric space with measure. A metric (or: distance) on a set $X$ will be denoted by $\rho$, and we will not remind the definition. The (open) ball of radius $r$ and centre $q$ in a metric space $(\Omega, \rho)$ is denoted

$$B_r(q) := \{\omega \in \Omega | \rho(q, \omega) < r\}.$$  

The family $\mathcal{B} = \mathcal{B}_\Omega$ of Borel subsets of a metric space $(\Omega, \rho)$ is the smallest family containing all the open balls and the entire set $\Omega$ and closed under complements and countable unions.

A (Borel) probability measure on the space $(\Omega, \rho)$ is a function $\mu : \mathcal{B}_\Omega \rightarrow [0,1]$ s.t. $\mu(\Omega) = 1$, and which is countably additive: for a sequence $B_1, B_2, \ldots$, of pairwise disjoint sets from $\mathcal{B}$, $\mu(\bigcup_i B_i) = \sum_i \mu(B_i)$.

A dataset however large is always a finite subset $X \subset \Omega$. It naturally inherits the metric $\rho|_X$ and in place of $\mu$ supports the normalized counting (also: empirical) probability

$$\mu^*_X(\cdot) := \frac{1}{|X|} \sum_{\omega \in X} \delta_\omega(\cdot),$$

where $\delta_\omega$ is the Dirac delta function at $\omega$. It is a probability measure on $X$ and naturally extends to a probability measure on $\Omega$.

We will perform our analysis on a sequence of (data) spaces that exhibit the concentration of measure phenomenon [Gro83], [Mil86] (Sect. V), a concept linked to what is called in [Sha06] workloads with vanishing variance. It is also in terms of this concentration of measure that we define the dimension $d$. To show that the above situation with a million clusters cannot happen (too often) we study the convergence of empirical probabilities to their true values using a result from Statistical Learning Theory [Vap98]. We introduce a property of a sequence of spaces which is sufficient to invoke this result.

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The performance of indexing schemes will therefore involve both \(d \to \infty\) and \(n \to \infty\). Search in sublinear time in \(n\) is an obvious goal:

\[ \text{querytime} = o(n). \]

where by querytime we mean the average time it takes for a similarity query to execute, time measured in distance computations.

Storage is also important, with at most polynomial storage allowed in theoretical analysis (though in practice even \(n^2\) may be too much):

\[ \text{storage} = n^{O(1)}. \]

For the pivot-based indexing scheme the storage will be measured by the number of distances stored.

We will follow an approach in the authoritative survey by [Ind04] and focus on a particular range for rate of growth for dimension \(d\), superlogarithmic but subpolynomial in \(n\):

\[
\begin{align*}
d &= \omega(\log n) & (1) \\
d &= n^{o(1)} & (2)
\end{align*}
\]

This choice of bounds is due to a case study of the Hamming cubes. Recall that the Hamming cube \(\Sigma^d\) of dimension \(d\) is the set of all binary sequences of length \(d\), and the distance between two strings is just the number of elements they don’t have in common divided by \(d\):

\[ \rho(x, y) = \frac{\sum_{i=1}^{d} |x_i - y_i|}{d} \]

(the normalized Hamming distance).

In the case where \(d\) grows slowly, \(d = O(\log n)\), all possible queries can be pre-computed and stored without breaking the polynomial storage requirement. Hence the lower bound. The upper bound results from the observation that if \(d\) grew so fast that \(n = q^{O(1)}\), a sequential scan would be polynomial in \(d\) and so acceptable.

Summarizing: The goal of finding a scalable index is to find polynomial (preferably degree less than 2) \(n\) storage algorithm that allows search in polynomial \(d\) time.

This stands in contrast to the curse of dimensionality conjecture, as stated in [Ind04]:

If \(d = \omega(\log n)\) and \(d = n^{o(1)}\), any sequence of indexes built on a sequence of datasets \(X_d \subset \Sigma_d\) allowing exact nearest neighbour search in time polynomial in \(d\) must use \(n^{\omega(1)}\) space.

The conjecture remains unproven in the case of general indexing schemes. The goal of this article is to show that at least for pivot-based indexes the above conjecture holds even in a strengthened form.
IV. Pivot-based indexing

We will focus on one class of indexing schemes, the pivot-based index (e.g. AESA, MVPT, BKT,...see [Cha01] and [Zez05]). The index is built using a set of pivots \( \{p_1 \ldots p_k\} \) from \( \Omega \), and consists of the array of \( n \times k \) distances
\[
\rho(x, p_i), \quad 1 \leq i \leq k, \quad x \in X.
\]
Given a range query with radius \( r \) and centre \( q \), the \( k \) distances \( \rho(q, p_1) \ldots \rho(q, p_k) \) are computed so that \( \rho(q, x) \) can be lower-bounded by the triangle inequality:
\[
\rho(q, x) \geq \sup_{1 \leq i \leq k} |\rho(q, p_i) - \rho(x, p_i)|.
\]
It is useful to think of a new distance function,
\[
\rho_k(q, x) := \sup_{1 \leq i \leq k} |\rho(q, p_i) - \rho(x, p_i)|.
\]
The fact that \( \rho(q, x) \geq \rho_k(q, x) \) can be used to discard all \( x \) satisfying \( \rho_k(q, x) > r \). For the remaining points, the algorithm will verify if \( \rho(q, x) \leq r \). If it is true, the point is returned.

We will only analyze range queries; \( k \)-nearest neighbour queries can always be simulated by a range query of suitable radius [Zez05].

For a query centre \( q \) denote by \( C_q \) all the points of \( X \) satisfying \( \rho_k(q, x) > r \), i.e. all the elements to be discarded. Making \( C_q \) large is the primary way of cutting the cost of search in our cost model. Of course we can achieve this trivially with a very large number of pivots. This will defeat the purpose however as
\[
\text{Cost of range search} = k + |X \setminus C_q|
\]
The most often used solution is to keep adding pivots as long as it is found experimentally to decrease the cost of search. If \( k \) is small, on the order of \( \log n \) (as often space limitations require), the most important component of cost becomes the size of \( X \)
\( C_q \) and this is where the choice of pivots would seem to matter. Various approaches to pivot selection have been investigated in [Bus03]. The empirical results seem to suggest that a moderate reduction in the number of distance computations can be achieved, although the relative improvement drops with increasing dimension.

Remark IV.1 (The number of pivots \( k \)). There are indexing schemes, like AESA [Zez05] where \( k = n \). However, in many situations \( n^2 \) storage is not practical, and it has even been argued that under certain assumptions the optimal number of pivots is on the order of \( \ln n \) [Cha01]. It is also true that the query algorithm we analyze has complexity at least \( k \) so only schemes with \( k = o(n) \) can claim to beat the curse of dimensionality.

V. Concentration of measure

Perhaps the most compelling way to describe the concentration of measure phenomenon is to draw a picture. We will attempt to draw the (surface of the) unit sphere \( S^d \) for various \( d \), by sampling points and projecting them onto a flat surface. Any orthogonal projection, say taking the first 2 coordinates, will give the picture similar to that in Figure 1. Under the sampling approach, it appears that high dimensional spheres are “small” even if we know their diameter to be a constant irrespective of \( d \).

![Figure 1. Projection of randomly sampled spheres of various dimensions d=10, 20, 50, 100](image)

This phenomenon is observed in a much greater variety of situations and formalized as follows. Given a metric space \((\Omega, \rho)\), define the \( \epsilon \)-neighborhood \( A_\epsilon \) of \( A \subset \Omega \) as
\[
A_\epsilon = \{ \omega \in \Omega | \rho(\omega, a) < \epsilon \text{ for some } a \in A \}.
\]

Definition V.1. The concentration function \( \alpha = \alpha_\Omega \) of a metric space with measure \((\Omega, \rho, \mu)\) is defined as
\[
\alpha(0) = 1/2, \quad \alpha(\epsilon) = \sup \{ 1 - \mu(A_\epsilon) | A \subset \Omega, \mu(A) \geq \frac{1}{2} \}, \quad \epsilon > 0.
\]

To put it less formally, we are trying to measure how much of the space remains after “fat” is added to a somewhat large set in the form of an \( \epsilon \) neighborhood. When very little remains, we say that the concentration of measure takes place.

Example V.1. The spheres \( S^d \) in \( \mathbb{R}^{d+1} \), taken with the geodesic or Euclidian distance and the normalized invariant measure, produce a concentration function bounded as
follows \cite{Mil86}:
\[
\alpha_n(\epsilon) \leq e^{-(d-1)\epsilon^2/2}.
\]

In this case an exact expression for the concentration function is known \cite{Mil86}, based on the fact that the half-sphere, among all subsets of measure at least 1/2, will always produce the smallest \(\epsilon\)-neighborhood, no matter the \(\epsilon\). A plot of the resulting concentration functions, for several values of \(d\), appears in Figure 2.

**Definition V.2.** A sequence of spaces \((\Omega_d)_{d=1}^{\infty}\) is a normal Lévy family \cite{Mil86} if \(C, c > 0\) exist such that
\[
\alpha(\epsilon) < Ce^{-c\epsilon^2d}.
\]

**Example V.2.** The Balls \(\mathbb{B}^d\), taken with the Euclidean distance and the uniform probability measure (\(d\)-dimensional Lebesgue), form a normal Lévy family.

**Example V.3.** The Hamming Cubes \(\Sigma^d\) form a normal Lévy family under the normalized Hamming metric and the uniform measure.

The concentration of measure can be equivalently described in terms of Lipschitz functions. Recalling that a function \(f : \Omega \rightarrow \mathbb{R}\) is \(1\)-Lipschitz if
\[
\forall x, y \in \Omega, \ |f(x) - f(y)| \leq \rho(x, y).
\]

Recalling further that a median of function \(f : (\Omega, \rho, \mu) \rightarrow \mathbb{R}\) is any number \(M\) satisfying:
\[
\mu\{\omega | f(\omega) \leq M\} \geq 1/2 \text{ and } \mu\{\omega | f(\omega) \geq M\} \geq 1/2.
\]

It is then relatively straightforward to prove:

**Theorem V.3 (Cf. \cite{Mil86}).** For a \(1\)-Lipschitz function \(f\) defined on space \((\Omega, \mu, \rho)\):
\[
\forall \epsilon > 0, \ \mu\{\omega | f(\omega) - M | > \epsilon\} < 2\alpha(\epsilon).
\]

The relevance of concentration of measure in indexing is noted in \cite{Pes00}. Observe that
\[
\rho(\cdot, \cdot) : \Omega \rightarrow R : \omega \mapsto \rho(\omega, p)
\]
is \(1\)-Lipschitz for any \(p\) and in particular a pivot. Hence Theorem V.3 can be applied to obtain a bound on the deviation from the median \(M = M_p\) of function \(\rho(\cdot, p)\):
\[
\forall r > 0, \ \mu\{\omega | |\rho(\omega, p) - M| > r\} < 2\alpha(r).
\]

We combine these statements for all pivots \(p_i\):
\[
\forall r > 0, \ \mu\{\omega | \sup_{1 \leq i \leq k} |\rho(\omega, p_i) - M_i| > r/2\} < 2k\alpha(r/2),
\]
as the probability of the union can always be upperbounded by the sum of the probabilities. We note that no assumptions about independence are used: the sequence \(\{p_i\}\) can be chosen in any way. Next, for all query centres \(q\) except a set of measure \(< 1 - \alpha(r/2)\):
\[
\forall r > 0, \ \mu\{\omega | \sup_{1 \leq i \leq k} |\rho(\omega, p_i) - \rho(q, p_i)| > r\} < 2k\alpha(r/2).
\]

We could introduce a set
\[
C_q = \{\omega | \rho_k(q, \omega) > r\}
\]
and think of \(C_q\) as the observation of \(C_q\) under \(\mu\). To recap: for a randomly chosen query centre and each query radius \(r > 0\), with probability \(> 1 - \alpha(r/2)\),
\[
\mu(C_q) < 2k\alpha(r/2).
\]

**Remark V.4.** We point out that Theorem V.3 applied to the distance function \(\rho\) gives a bound on the variance of \(\rho(\cdot, \rho)\). This, together with a “uniformity of view” type assumption as in [Cha01b] leads us to conclude that the variance of \(\rho(\cdot, \cdot)\) converges to zero in Lévy families. This argument can be formalized to demonstrate the connection to the assumption of vanishing variance on the sequence of data spaces made in \cite{Sha06}. In our view that assumption is just a variation on concentration of measure. The differences lie in certain technical details, like the division by expectation of \(\rho(\cdot, \cdot)\) in \cite{Sha06}. Here we simply avoid the issue by normalizing spaces so that the expectation of \(\rho(\cdot, \cdot)\) tends to a constant. This normalization also fixes the problem of distance to nearest neighbour (e.g. \cite{Web98}) as we demonstrate in the next section.

**VI. RADIUS OF QUERIES IN LÉVY FAMILIES**

In our asymptotic analysis, we would like to normalize spaces so that the median distance between two points stays about the same. Here we will extract consequences for the typical radius of a query – which we will assume to be the distance to the nearest neighbour of query centre.

**Lemma VI.1 (M. Gromov, V.D. Milman).** \cite{Gro83} Let \((\Omega, \rho, \mu)\) denote a metric space with measure and \(\alpha\) its concentration function. Then if \(A \in \Omega\) is such that \(\mu(A) \geq \alpha(\gamma)\) for some \(\gamma > 0\), it implies that \(\mu(A_r) \geq 1/2\).

**Theorem VI.2.** Let \((\Omega_d, \rho_d, \mu_d, X_d)_{d=1}^{\infty}\) be a sequence of metric spaces with measure, forming a Lévy family, together with i.i.d. samples \(X_d\). Assume that \(n = n_d = |X_d| = \varphi(n_d)\). Furthermore, if \(M_d\) denotes the median value of \(\{\rho_d(\omega_1, \omega_2) | \omega_1 \in \Omega_d\}\), we assume that \(M_d = \Theta(1)\), that is, for some fixed \(c_1, c_2 > 0\), \(\forall d, c_1 < M_d < c_2\).

Let \(\rho_{NN}^d(\omega)\) denote the distance to the nearest neighbour of \(\omega \in \Omega_d\) in \(X_d\). Define \(m_d\) to be the median of...
where \( \rho^{(NN)}_d(\omega) \). Then there exists some \( c_3 > 0 \) and some \( D \) such that for all \( d \geq D \), \( m_d > c_3 \).

Proof: Assume the conclusion fails, then without loss of generality and proceeding to subsequence if necessary, \( m_d \to 0 \). By definition of \( m_d \), we know that for any \( d \),

\[
\mu_d \left( \bigcup_{x \in X} B_{m_d}(x) \right) \geq \frac{1}{2}.
\]

It follows that

\[
n_d \sup_{\omega \in \Omega_d} \mu_d (B_{m_d}(\omega)) \geq \frac{1}{2},
\]

and so we can find for any \( d \) a point \( \omega_d \in \Omega_d \) such that

\[
\mu_d (B_{m_d}(\omega_d)) \geq \frac{1}{2n}.
\]

If we denote by \( \alpha_d \) the concentration functions of our spaces \( \Omega_d \) we know by assumption the existence of \( C, c > 0 \) s.t.

\[
\forall d, \alpha_d(\epsilon) \leq Ce^{-c\epsilon^2}d = d^{-o(1)}.
\]

Hence we can find \( d' \) s.t. \( \alpha_d(\gamma) < 1/2n_{d'} \) and \( m_{d'} < c_1/8 \), where \( \gamma = c_1/8 \) as well. By lemma [VI.1]

\[
\mu_{d'} (B_{m_{d'}}(\omega_{d'})) \gamma \geq \frac{1}{2}.
\]

It then follows that

\[
\mu_{d'} \left( (B_{m_{d'}}(\omega_{d'})) \gamma \right) \geq 1 - Ce^{-c\gamma^2d'}
\]

that is, since \( m_{d'} + 2\gamma < 3c/8 \),

\[
\mu_{d'} (B_{3c/8}(\omega_{d'})) \geq 1 - Ce^{-c\gamma^2d'}.
\]

But diameter \( (B_{3c/8}(\omega_{d'})) \leq 3c_1/4 \), so in \( \Omega_{d'} \times \Omega_{d'} \) the measure of the set of points \( (\omega_1, \omega_2) \) for which \( \rho_{d'}(\omega_1, \omega_2) < c_1 \) is at least

\[
\left( 1 - \frac{1}{2n_{d'}} \right)^2,
\]

obviously contradicting \( M_{d'} > c_1 \).

This result frees us from having to consider a radius that vanishes as \( n, d \) go to infinity. With this achieved, let us recap our goal: to show that a large proportion of queries are slow, something along the lines of:

\[
\text{median}_{q,p,r} \left( \mu_n (C_{q,p_1...p_k(r(n))} \right) \to 0 \text{ as } n, d \to \infty,
\]

where the median is taken over all the queries under consideration: any \( q \in \Omega_d \) and any \( r \) at least as large as the distance to the nearest neighbour of \( q \) in \( X \). As well, for each \( d \) and \( n = n_d \) we would like to also consider all possible pivot-based index schemes (as long as \( k \) is within certain ranges we will specify later). So far we have shown, although the proof was just sketched (and with the detail about \( k \) left out) that

\[
\text{median}_{q,p,r} (\mu (C_{q,p_1...p_k(n)}, r(n))) \to 0 \text{ as } n, d \to \infty
\]

(5)

What we need is to find out when (5) implies (4). To do so we will summon the powerful machinery of statistical learning theory.

VII. Statistical Learning Theory

Statistical learning theory has already been used in the analysis and design of indexing algorithms [Kle97] and is a vast subject. We will just focus on the generalization of the Glivenko-Cantelli theorem due to Vapnik and Chervonenkis.

Theorem VII.1 (Glivenko-Cantelli). Given sample \((X_1,X_2,...,X_n)\) distributed i.i.d. according to any measure \( \mu \) on \( \mathbb{R}^n \), we have:

\[
\sup_{r \in \mathbb{R}} |\mu_n(-\infty,r] - \mu(-\infty,r]| \to 0,
\]

where

\[
A = \{(-\infty,r]|r \in \mathbb{R}\},
\]

which makes more apparent a path for extension: to generalize to other collections of subsets \( A \).

A collection \( A \) “colours” the sample \( X \) as follows. Each \( A \in A \) will assign 1 to \( X_i \) if \( X_i \in A \), and 0 otherwise. We denote by \( N(X) \) the number of such different colourings of \( X \) generated by all \( A \in A \). Clearly \( N(X) \leq 2^n \). What is surprising is that in many situations, despite a seemingly rich \( A \), we have \( N(X) \ll 2^n \).

Definition VII.2. The growth function \( G = G_A \) of a family \( A \) is defined by

\[
G(n) = \ln \sup_{|X|=n} N(X).
\]

It is independent of \( \mu \) and the choice of sample \( X \).

There are two cases to consider for an upper bound for the growth function [Vap98]:

- for all \( n \), \( G(n) = n \ln 2 \)
- or, for the largest \( \Delta \) such that \( G(\Delta) = \Delta \ln 2 \),

\[
G(n) \left\{ \begin{array}{ll}
= n \ln 2 & \text{if } n \leq \Delta \\
\leq \Delta (1 + \ln(n/\Delta)) & \text{if } n > \Delta
\end{array} \right.
\]

This \( \Delta \) is the so-called VC dimension and it turns out that its finiteness is a necessary and sufficient condition for (6). The rate of convergence is as follows ([Vap98] p.148):
Theorem VII.3. [Vapnik–Chervonenkis] For a collection \( A \) of subsets of \( \Omega \), of finite VC dimension \( \Delta \), and any measure \( \mu \) on \( \Omega \), we have that for any \( \varepsilon > 0 \),

\[
P \left[ \sup_{A \in A} \left| \mu_n(A) - \mu(A) \right| > \varepsilon \right] < 4 \exp \left( \frac{\Delta(1 + \ln(2n/\Delta))}{n} - \left( \varepsilon - \frac{1}{n} \right)^2 \right) n.
\]

The convergence is eventually like \( \exp(-\varepsilon^2 n) \), which is again a fast rate of convergence. Since no information about the measure \( \mu \) is incorporated, the left side can be replaced by its supremum taken over all possible probability measures on the domain \( \Omega \).

A natural restatement of these results is to ask how big does the sample size \( n \) have to be for the expression on the left to be less than some \( \eta > 0 \). Solving for \( \eta \) and the use of some technical inequalities (cf e.g. [Men03]) yields:

\[
n \geq \frac{128}{\varepsilon^2} \left( \Delta \log \frac{2e^2}{\varepsilon} + \log \frac{8}{\eta} \right).
\]

Calculations of VC dimension have been done for various objects (e.g. [Dud84], [Vap98], [Dev97]): The VC dimension of half-spaces \( \{ x \in \mathbb{R}^d | x \cdot v \geq b \} \) in \( \mathbb{R}^d \) is \( d+1 \). The VC dimension of all open (or closed) balls in \( \mathbb{R}^d \) is also \( d+1 \). Axis-aligned rectangular parallelepipeds in \( \mathbb{R}^d \), i.e. sets of form \( [a_1, b_1] \times [a_2, b_2] \times \ldots \times [a_d, b_d] \) have a VC dimension of \( 2d \).

Our interest is in calculating the VC dimension of all possible set of form \( C_q \), the collection of which for a fixed \( k \) we denote:

\[
A = A_k = \{ C_{q,p_1,...,p_k(n),r(n)} | q \in \Omega, p_1 \in \Omega, r > 0 \}
\]

As

\[
C = \{ \omega : \sup_i \| \omega - p_i \| - \| q - p_i \| > r \} = (\bigcap_i \{ \omega : \| \omega - p_i \| - \| q - p_i \| \leq r \})^c,
\]

we can proceed through several steps. A set of the form

\[
\{ \omega : \| \omega - p_i \| - \| q - p_i \| \leq r \}
\]

is a “spherical shell,” and an intersection of shells is an intersection of sets from \( A \cup A^c \), where \( A \) is the collection of all balls. It is easy to show that given a collection \( A \) the complement collection \( A^c = \{ A^c | A \in A \} \) has the same VC dimension. The VC dimension of balls was quoted above as \( d+1 \), hence the VC dimension of complements of balls is \( d+1 \) as well. The VC dimension of the union of the two collections is

\[
(d+1) + (d+1) + 1 = 2d + 3,
\]

as a consequence of a general result [Vid03]: If a collection \( A \) has VC dimension \( \Delta_A \) and a collection \( B \) has VC dimension \( \Delta_B \), the union \( A \cup B \) has VC dimension at most \( \Delta_A + \Delta_B + 1 \).

A result for intersection of sets is mentioned in [Blu89]:

Lemma VII.4. For \((\Omega, \rho) = (\mathbb{R}^d, L^2)\), an upper bound on the VC dimension of \( A_{\cap \rho} \), composed of k-fold interesections of elements of a family \( A \) of VC dimension \( \Delta \) is \( 2\Delta k \ln(3k) \).

Hence we can conclude that the VC dimension of \( A_k \) for the case \( \Omega \subset \mathbb{R}^n \) is bounded by

\[
2(2d+3)(2k)\ln((3)(2k)) = k(8d + 12) \ln(6k),
\]

where \( k \) is the number of pivots.

Another example comes from considering the Hamming cube. As there are \( 2^d \) points in a \( d \)-dimensional Hamming cube, and at most \( d \) different radii, at most \( d2^d \) different balls exist. We know from e.g. [Blu89] that if the class \( A \) is finite, its VC dimension is bounded by \( \log_d |A| \). Disregarding the small leftover term, the VC dimension for balls in the Hamming cube is about \( d \).

Summarizing:

Theorem VII.5. Let us denote by \( \Delta \) the VC dimension of collection \( A_k \) as defined in equation (8). Then upper bounds on \( \Delta \), depending on the metric space, are as follows:

- For \((\mathbb{R}^d, L^2)\), \( \Delta \leq k(8d + 12) \ln(6k) \).
- For \((\mathbb{R}^d, L^\infty)\), \( \Delta \leq k(16d + 4) \ln(6k) \).
- For \((\Omega^d, \rho)\), \( \Delta \leq k(8d + 8 \log_d d + 4) \ln(6k) \).

VIII. MAIN RESULT

Theorem VIII.1. Consider a sequence of metric spaces \((\Omega_d, \rho_d)\), where \( d = 1, 2, 3, \ldots \) and the VC dimension of closed balls in \((\Omega_d, \rho_d)\) is \( O(d) \). Assume every \( \Omega_d \) supports a Borel probability measure \( \mu_d \) so that for some \( C, \varepsilon > 0 \) the concentration functions \( \alpha_d \) of \((\Omega_d, \rho_d, \mu_d)\) satisfy

\[
\forall \varepsilon > 0, \quad \alpha_d(\varepsilon) \leq Ce^{-\varepsilon^2 d}.
\]

Select for each \( d \) an i.i.d. sample \( X_d \) of size \( n_d \) from \( \Omega_d \), according to \( \mu_d \), where the sample size \( n_d \) satisfies \( d = \omega(\log n_d) \) and \( d = n_d^{o(1)} \). Suppose further for every \( d \) a pivot index for similarity search is built using \( k \) pivots, where

\[
k = o(n_d/d).
\]

Fix arbitrarily small \( \varepsilon, \eta > 0 \). Suppose we only ask queries whose radius is equal or greater to the distance to nearest neighbour of query centre \( q \in \Omega_d \) in \( X_d \).

Then there exists a \( D \) such that for all \( d \geq D \), the probability that at least half the queries on dataset \( X_d \) take less than \((1 - \varepsilon)n_d \) time is less than \( \eta \).

Furthermore, if we allow the likelihood \( \eta \) to depend on \( d \), we can pick \( n_d \) so that the above holds true and

\[
\lim_{D \to \infty} \prod_{d=D}^{\infty} (1 - \eta_d) = 1.
\]
We emphasize that this result is independent of the selection of pivots.

Sketch of a proof: From Eq. (3) we know that, for a vast majority of query centres \( q \),
\[
\mu(C_q) \leq M_2ke^{-dr^2},
\]
where \( M_2 \) is some constant.

We will sacrifice a certain number of sets of form \( C_q \) so that \( r \) can be considered a constant (see section VII); we will proceed with at least half the queries having radius \( r \) above a constant independent of \( d \). Hence the quantities that vary in \( d \) are \( n \) and \( k \). Since \( d \) is superlogarithmic in \( n \),
\[
\forall c > 0, d > c \log n \\
\Rightarrow \forall c > 0, \exp(-d) < \exp(-c \log n) \\
\Rightarrow \forall c > 0, \exp(-d) < cn.
\]

So \( e^{-dr^2} = o(n) \), and hence \( \mu(C_q) = o(n) \). In fact this holds for at least half the queries \( q \) simultaneously, so:
\[
\text{median sup}_{C_q} \mu(C_q) = o(n).
\]

From the previous section, we know that only for large values of \( n \) will empirical measures be close (up to \( \varepsilon \)) to actual measures with likelihood \( (1-\eta) \). The lower bound on \( n \) then naturally depends on \( \varepsilon, \eta \) but also on the VC dimension \( \Delta \) of the collection \( A_k \).

Let us fix \( \varepsilon = 1/2 \) and assume \( \eta \) is bounded by some value less than 1. Then by pooling all constants, including \( \varepsilon \) and \( \eta \) but not \( \Delta \) we can rewrite expression (7) as:
\[
n \geq M_1 \Delta,
\]
where \( M_1 > 1 \). What we would like to avoid is to have the right part of this expression grow linearly in \( n \). We know an upper bound on \( \Delta \) depends on \( k \) and \( d \) as established in Theorem VII.5. As our concern is for asymptotic behaviour we will simplify this bound to \( kd \log k \).

Combining \( d = o(n) \) with the asymptotic condition on \( k \), we conclude that:
\[
\Delta = o(n),
\]
and hence asymptotically we know that the right side of expression (10) falls (much) under \( n \). Therefore we are able to conclude:
\[
P(\sup_{C_q} |\mu_{q}(C_q) - \mu(C_q)| > \varepsilon) < \eta,
\]
which, combined with \( \varepsilon = 1/2 \) and median sup_{C_q} \mu(C_q) = o(n), gives the first part of the result.

According to expression (7),
\[
\eta \geq \exp\left( \Delta \log \left( \frac{2\varepsilon^2}{\varepsilon} \right) + \log 8 - \frac{\varepsilon^2 n}{128} \right) = \exp(-d^{o(1)}).
\]

Assuming independent choices of the datasets \( X_d \), and assuming that for each \( d \) the probability of an event is at least \( 1 - \eta_d \), we aim to prove that
\[
\lim_{D \to \infty} \prod_{d=D}^{\infty} (1 - \eta_d) = 1.
\]

As \( \eta_d \) goes to 0 at least as fast as \( e^{-d} \), it is enough to show that
\[
\lim_{D \to \infty} \prod_{d=D}^{\infty} (1 - e^{-d}) = 1.
\]

Observing [Ash71] that for any sequence \( 0 \leq \eta_d \leq 1 \),
\[
1 - \sum_{d=1}^{N} \eta_d \leq \prod_{d=1}^{N} (1 - \eta_d) \leq \exp \left( \sum_{d=1}^{N} -\eta_d \right),
\]
we can extend this, for any \( D \) to:
\[
1 - \sum_{d=D}^{\infty} \eta_d \leq \prod_{d=D}^{\infty} (1 - \eta_d) \leq \exp \left( \sum_{d=D}^{\infty} -\eta_d \right).
\]

Summing the geometric series, we obtain Eq. (12).

A. Conclusion

We have established a rigorous asymptotically linear lower bound on the expected average performance of the optimal pivot-based indexing schemes for similarity search in datasets randomly sampled from domains whose dimension goes to infinity. The examples given above of the various spaces exhibiting normal concentration of measure should convince the reader that many of the most naturally occuring domains and measure distributions are such.

This is not the first lower bound result for pivoting algorithms for exact similarity search. A specific lower bound for pivot-based indexing already mentioned above is that of [Cha01b]:
\[
\tilde{d} \log n.
\]

This result assumes that \( k = \Theta(\log n) \). Furthermore and more importantly, the pivot selection is assumed to be random, as opposed to our (much stronger) bound that is applicable to any pivot selection technique.

Other, more general asymptotic analyses considering more classes of indexing schemes [Web98, Sha06] fix \( n \) or in the case of [Web98] also fail to distinguish between the dataset and the dataspace making results appear stronger than they actually are.

The aim in [Sha06] was to demonstrate that
\[
\frac{E(\text{cost})}{n} \to 1
\]
which came at the expense of any results on the rate of convergence. We chose instead to prove a weaker result, with convergence to some number close to 1/2 but with estimates on the rate of convergence.
It should be assumed that the hypotheses of our paper are universal. Rather, our theoretical analysis confirms that at least in some settings, the curse of dimensionality for pivot-based schemes is indeed in the nature of data. Probably a more realistic situation from the viewpoint of applications would be that of an intrinsically low dimensional dataset contained in a high-dimensional domain, and performing an asymptotic analysis of various indexing schemes in this setting is an interesting open problem.

REFERENCES

[Ash71] Ash, R.B. (1971) Complex Variables. Academic Press.

[Bey99] Beyer, K., Goldstein, J., Ramakrishnan, R., Shaft, U. (1999) When is “Nearest Neighbour” meaningful? Lect. Notes in Comp. Sci., vol. 1540, 217–235

[Blu89] Blumer, A., Ehrenfeucht, A., Haussler, D., Warmuth, M.K. (1989) Learnability and the Vapnik-Chervonenkis dimension. *Journal of the ACM*, 36, 929–965.

[Bus03] Bustos, B., Chávez, E., Navarro, G (2003) Pivot selection techniques for proximity searching in metric spaces. Pattern Recognition Letters, 24-14, 2357–2366.

[Cia97] Ciaccia, P., Patella, M., Zezula, P. (1997) M-tree: An efficient access method for similarity search in metric spaces. Proc. VLDB 1997: pp426-435

[Cia98] Ciaccia, P., Patella, M., Zezula, P. (1998) A cost model for similarity queries in metric spaces. Proc. 17th ACM SIGACT-SIGMOD-SIGART Symposium on Principles of Database Systems.

[Cha01] Chávez, E., Navarro, G. Baeza-Yates, R. & Marroquín, J. L. (2001). Searching in metric spaces. ACM Computing Surveys, 33, 273–321.

[Cha01b] Chávez, E., Navarro, G. (2001). Towards measuring the searching complexity of metric spaces. Proceedings of ENC’01, 969–978.

[Cha05] Chávez, E., Navarro, G. (2005). A compact space decomposition for effective metric indexing. Pattern Recognition Letters, v.26, issue 9, pp 1363 – 1376

[Cha05] Clarkson, K.L. (2005) Nearest-Neighbor Searching and Metric Space Dimensions. Nearest-Neighbor Methods for Learning and Vision: Theory and Practice, MIT Press, 2006.

[Dev97] Devroye, L., Györfi, L., Lugosi, G. (1997) A Probabilistic Theory of Pattern Recognition. Springer

[Dud84] Dudley, R.M. (1984). A Course on Empirical Processes. Lecture Notes in Math. Springer, New York, 1984

[Gro83] Gromov, M., Milman, V.D. (1983). A topological application of the isoperimetric inequality. Amer. J. Math. 105, 843–854.

[Heg01] Hegland, M. (2001) Data mining techniques. Acta Numerica, 2001 pp313-355

[Ind04] Indyk, P. (2004). Ch. 39 of Handbook of Discrete and Computational Geometry, Goodman, J.E., O’Rourke, J., eds., CRC Press.

[Kle97] Kleinberg, J. (1997) Two algorithms for nearest-neighbor search in high dimensions. Proc. 29th ACM Symposium on Theory of Computing.

[Men03] Mendelson, S. (2003) A few notes on statistical learning theory. Advanced Lectures in Machine Learning LNCS 2600, 1–40. Springer

[Mil86] Milman, V.D., Schechtman, G. (1986) Asymptotic theory of finite dimensional normed spaces. Lecture Notes in Mathematics.

[Pes00] Pestov, V. (2000). On the geometry of similarity search: dimensionality curse and concentration of measure. *Inform. Process. Lett.* 73, 47–51.

[Pes08] Pestov, V. (2008). An axiomatic approach to intrinsic dimension of a dataset. Neural Networks 21, 204–213.

[Sha06] Shaft, U., Ramakrishnan, R. (2006) Theory of nearest neighbors indexability . ACM Transactions on Database Systems, Volume 31 , Issue 3, pp 814 – 838.

[Vap98] Vapnik, V. (1998) Statistical Learning Theory. Wiley series on adaptive and learning systems for signal processing, communications and control.

[Web98] Weber, R., Schek, Hans-J., Blott, S. (1998) A Quantitative Analysis and Performance Study for Similarity-Search Methods in High-Dimensional Spaces Proceedings of the 24rd International Conference on Very Large Data Bases, pp194-205.

[Zee05] Zezula, P., Amato, G., Dohnal, V., Batko, M. (2005) Similarity search: the metric space approach. *Springer series: advances in database systems*, vol 32.