New Instability Results for High Dimensional Nearest Neighbor Search

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Abstract

Consider a dataset of n(d) points generated independently from \mathbb{R}^d according to a common p.d.f. f_d with $support(f_d) = [0,1]^d$ and $sup\{f_d([0,1]^d)\}$ growing sub-exponentially in d. We prove that: (i) if n(d) grows sub-exponentially in d, then, for any query point $\vec{q}^d \in [0,1]^d$ and any $\epsilon > 0$, the ratio of the distance between any two dataset points and \vec{q}^d is less that $1 + \epsilon$ with probability $\to 1$ as $d \to \infty$; (ii) if $n(d) > [4(1 + \epsilon)]^d$ for large d, then for all $\vec{q}^d \in [0,1]^d$ (except a small subset) and any $\epsilon > 0$, the distance ratio is less than $1 + \epsilon$ with limiting probability strictly bounded away from one. Moreover, we provide preliminary results along the lines of (i) when $f_d = N(\vec{\mu}_d, \Sigma_d)$.

Key words: information retrieval, curse of dimensionality

1. Introduction

Nearest neighbor search on high-dimensional data is a difficult (and well-studied) problem, in part, because many commonly used distance functions can exhibit greatly different behavior in low versus high-dimensional spaces – a phenomenon often referred to as the "curse of dimensionality". In an effort to rigorously analyze this phenomenon, Beyer et al. [3] defined a nearest neighbor query with respect to a reference query point $\vec{q}^d \in \mathbb{R}^d$ as unstable if all of the points in the dataset are nearly the same distance from \vec{q}^d . In this event, the query can be thought meaningless since there is little reason to return any one point over another (see figure 2 in [3]). Beyer et al. (then later others [4], [11]) established sufficient conditions on the data generation distributions and dataset sizes under which the probability of query instability approaches one as $d \to \infty$. Such conditions provide useful insight into how the curse can be mitigated or must be tolerated as unavoidable. We develop a new set of sufficient conditions which improve upon the

current ones – see sub-sections 1.2 and 1.3 for a description of our contributions and their relationship to the literature.

1.1. Notations and Definitions

Given $n(.): \mathbb{N} \to \mathbb{N}$, we represent a d-dimensional, size n(d) dataset with i.i.d. random vectors $\vec{Y}_1, \ldots, \vec{Y}_{n(d)}$ having common p.d.f. f_d . Let $support(f_d)$ denote the topological closure of $\{\vec{y} \in \mathbb{R}^d : f_d(\vec{y}) > 0\}$. Given posative real number p, the distance between a pair of points $\vec{z}, \vec{w} \in \mathbb{R}^d$ is defined as: $||\vec{z} - \vec{w}||_p = \left[\sum_{j=1}^d |z_j - w_j|^p\right]^{1/p}$. Given $\epsilon > 0$, the probability of a nearest neighbor query $\vec{q}^d \in support(f_d)$ being unstable is $P_{d,n(.),\vec{q}^d} = Pr\left[\max_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p\} \le (1+\epsilon) \min_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p\}\right]$.

The space of all possible query point sequences is $\prod_{d=1}^{\infty} support(f_d)$. We say that data distribution sequence $\{f_d: d=1,2,\cdots\}$ and dataset size function n(.) admit nearest neighbor instability if for any $\epsilon>0$ and any query point sequence $\{\vec{q}^d\}\in\prod_{d=1}^{\infty} support(f_d)$, it is the case that $\lim_{d\to\infty}P_{d,n(.),\vec{q}^d}=1$. We say that $\{f_d\}$ and n(.) strongly fail to admit nearest neighbor instability if there exists $\zeta<1$ and a "large" $\mathcal{Q}\subseteq\prod_{d=1}^{\infty} support(f_d)$, such that for any $\epsilon>0$ and for any $\{\vec{q}^d\}\in\mathcal{Q}$, it is the case that $\lim_{d\to\infty}P_{d,n(.),\vec{q}^d}<\zeta$. Let \mathcal{Q}^d denote the d^{th} component of \mathcal{Q} . We say that \mathcal{Q} is "large" if for any $0\leq\omega<1$, it is the case that, $\lim_{d\to\infty}\frac{\omega^d Volume(support(f_d))}{Volume(\mathcal{Q}^d)}=0$. Note, if $support(f_d)=[0,1]^d$, this last condition is equivalent to $\lim_{d\to\infty}\frac{Volume([0,\omega]^d)}{Volume(\mathcal{Q}^d)}=0$.

A function $g: \mathbb{N} \to \mathbb{N}$ is said to grow sub-exponentially if $\lim_{d\to\infty} \frac{\log(g(d))}{d} = 0$. A sequence of functions, $f_d: \mathbb{R}^d \to \mathbb{R}$; $d = 1, 2, \ldots$, is said to be bounded above sub-exponentially if, for all d, $\sup\{f_d(\mathbb{R}^d)\} \leq g(d)$.

1.2. Our Contributions

For any $\{f_d\}$ bounded above sub-exponentially and $support(f_d) = [0,1]^d$, we prove the following: (i) if n(.) grows sub-exponentially, then nearest neighbor instability is admitted; (ii) if $n(d) > [4(1+\epsilon)]^d$ for large d, then (with $p \ge 1$) instability strongly fails to be admitted. Moreover, we describe preliminary results toward establishing sufficient conditions under which $\{N(\vec{\mu}_d, \Sigma_d)\}$ admits instability.

1.3. Related Work

Beyer et al. [3] established sufficient conditions upon n(.) and $\{f_d\}$ for the admission of nearest neighbor instability. They proved that instability is admitted if n(.) is constant and $\{f_d\}$ satisfies: $\lim_{d\to\infty} Var\left[\frac{||\vec{Y}_1-\vec{q}^d||_p}{E[||\vec{Y}_1-\vec{q}^d||_p]}\right]=0$, for any $\{\vec{q}^d\}$ (the relative variance goes to zero). Pestov [11], proved that (Corollary 5.5) instability is admitted (except for a small set of query point sequences) if n(.) is sub-exponentially growing and $\{f_d\}$ satisfies three conditions, most notably, $\{f_d\}$ forms a normal Levy family as defined with respect to the "concentration of measure" phenomena. Francois et al. [4] proved that instability is admitted (with $\{\vec{q}^d\} = \{\vec{0}\}$) if n(.) is constant and each distribution in $\{f_d\}$ has i.i.d. attributes with mean and variance not dependent on d.

Our contributions significantly advance the above results as follows. Our sufficient conditions allow n(.) to grow with d (unlike Beyer et~al. and Francois et~al.), are quite broad (unlike Francois et~al. who require the data distributions to have i.i.d. attributes), and are easy to interpret (unlike Beyer et~al. or Pestov et~al. which leave open the question of which data distribution sequences satisfy the relative variance condition or normal Levy condition, respectively). Moreover, we provide results showing that the sub-exponential growth assumption on n(.) is strongly necessary: if n(.) grows exponentially, then instability fails to be admitted for a large space of query point sequences. Finally, we provide preliminary results toward establishing sufficient conditions for $\{N(\vec{\mu}_d, \Sigma_d)\}$. To our knowledge, the sufficient conditions for this distribution sequence remain unknown.

Aggarwal et al. [2] considered distance functions with p a positive integer and proved that, for constant n(.) = N and data distributions with i.i.d. attributes supported on (0,1), $C_p \leq \lim_{d\to\infty} \frac{E[\max_{i=1}^N ||\vec{Y}_i||_p - \min_{i=1}^N ||\vec{Y}_i||_p]}{d^{1/p-1/2}} \leq (N-1)C_p$, with C_p a constant not dependent on d. They argued that high-dimensional nearest neighbor behavior is sharply different for each of the following three types of distance functions: p=1, p=2, and $p\geq 3$. However, unlike our contributions, they do not provide sufficient conditions on instability and they make the restrictive i.i.d. data attribute assumption. Hsu and Chen [7] proved³ that, for constant n(.), the relative variance condition of Beyer is a necessary

¹They considered any non-negative distance function and did not restrict query points to reside in $support(f_d)$.

²He considered any metric distance function.

³They consider any non-negative distance function.

as well as a sufficient condition for instability admission. They go on to develop a basis for empirically testing whether instability is exhibited.

Shaft and Ramakrishnan [12] considered the related problem of analytically quantifying the inherent limits of nearest-neighbor indexing on high-dimensional data. They proved that, under conditions related to those in Beyer et~al., the performance of a broad class of index structures approaches that of linear scan as $d \to \infty$. In the stochastic geometry literature, Zanger [13] studied the behavior of a general class of clustering functions as $d \to \infty$ and established a connection to the concentration of measure phenomenon. A more broadly studied problem in this literature is the behavior of nearest neighbor structures as the dataset~size goes to infinity and d remains constant. For example, Penrose [10] considered data generated i.i.d. from a continuous p.d.f. with compact support (and "smooth" boundary) and showed that, as $N \to \infty$, the distance of any point to its k nearest neighbor converges, almost surely, to a constant not dependent on N.

A vast literature exists on the development of data structures and algorithms for nearest neighbor search, for brevity, see the discussion and citations in [7].

2. Instability Results

First we develop a lower-bound on $P_{d,n(.),\vec{q}^d}$ making no assumptions on $\{f_d\}$ or n(.). Define $\delta(\epsilon,p) = [(1+\epsilon)^p-1]/[(1+\epsilon)^p+1]$ and let $\gamma \geq 0$. If for all $1 \leq i \leq n(d)$, $\left|||\vec{Y}_i - \vec{q}^d||_p^p - \gamma\right| \leq \gamma \delta(\epsilon,p)$, then $\max_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p^p\} \leq \min_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p^p\} \frac{[1+\delta(\epsilon,p)]}{[1-\delta(\epsilon,p)]} = \min_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p^p\} (1+\epsilon)^p$. Thus, $\max_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p\} \leq \min_{i=1}^{n(d)} \{||\vec{Y}_i - \vec{q}^d||_p\} (1+\epsilon)$. Using this and the fact that $\vec{Y}_1, \dots, \vec{Y}_{n(d)}$ are i.i.d.,

$$P_{d,n(.),\vec{q}^d} \geq Pr\left[\forall i, \left| ||\vec{Y}_i - \vec{q}^d||_p^p - \gamma \right| \leq \gamma \delta(\epsilon, p) \right]$$

$$= \left(1 - Pr\left[\left| ||\vec{Y}_1 - \vec{q}^d||_p^p - \gamma \right| > \gamma \delta(\epsilon, p) \right] \right)^{n(d)}. \tag{1}$$

Our results are reduced to upper-bounding the probability that a sum of random variables, $||\vec{Y}_1 - \vec{q}^{tl}||_p^p$, deviates significantly from a fixed value γ . To our knowledge, developing a useful bound in the most general case is not possible. To get around this problem, we show how our assumptions on $\{f_d\}$ and n(.) allow the dependences between the components

of $(\vec{Y}_1 - \vec{q}^d)$ to be broken, and thus, open the door to applying standard concentration bounds (e.g. Hoeffding) on the r.h.s. of (1).

Assume $\{f_d\}$ is bounded above sub-exponentially and $support(f_d) = [0,1]^d$. Let U_1, \ldots, U_d be i.i.d. and distributed uniformly on [0,1]. Let S denote $\{\vec{y} \in [0,1]^d : |||\vec{y} - \vec{q}^d||_p^p - \gamma| > \gamma \delta(\epsilon, p)\}$. There exists sub-exponentially growing function $\beta(.)$ such that,

$$Pr\left[\left|||\vec{Y}_{1} - \vec{q}^{d}||_{p}^{p} - \gamma\right| > \gamma\delta(\epsilon, p)\right] = \int_{\vec{y} \in S} f_{d}(\vec{y})\partial\vec{y}$$

$$\leq \beta(d) \int_{\vec{y} \in S} \partial\vec{y}$$

$$= \beta(d)Pr\left[\left|\sum_{j=1}^{d} |U_{j} - q_{j}^{d}|^{p} - \gamma\right| > \gamma\delta(\epsilon, p)\right]$$

$$\leq \beta(d)2exp\left(\frac{-2\delta(\epsilon, p)^{2}\left[\frac{d}{(p+1)2^{p}}\right]^{2}}{d}\right).$$

The first equality and inequality follow from the fact that $support(f_d) = [0,1]^d$ and f_d is bounded above sub-exponentially, respectively. The second inequality follows from Theorem 2 of Hoeffding [6].⁴ Plugging this bound into the r.h.s. of inequality (1) yields an expression which goes to one as $d \to \infty$, due to the sub-exponential growth assumptions on n(.) and $\beta(.)$.

3. Dataset Size Assumption

Now we relax the assumption that n(.) grows sub-exponentially while still assuming that $\{f_d\}$ is bounded above sub-exponentially and $support(f_d) = [0,1]^d$. Suppose that, for large d, $n(d) > [4(1+\epsilon)]^d$. We further assume that $p \ge 1$. Our goal in this section is to show that $\{f_d\}$ and n(.) strongly fail to admit instability.

With $\gamma = \sum_{j=1}^{d} E[|U_j - q_j^d|^p]$, $X_j = |U_j - q_j^d|^p$, and $t = \left(\delta(\epsilon, p) \sum_{j=1}^{d} E[|U_j - q_j^d|^p]\right)/d$. Clearly t > 0. Also, since $support(U_j) = [0, 1]$ and $\vec{q}^d \in support(f_d) = [0, 1]^d$, then $0 \le |U_j - q_j^d|^p \le 1$. Finally, $E[|U_j - q_j^d|^p] = [(q_j^d)^{p+1} + (1 - q_j^d)^{p+1}]/(p+1)$ which, for $0 \le q_j^d \le 1$, obtains its minimum of $1/(p+1)2^p$ at $q_j^d = 1/2$.

Fix $99/100 < \zeta < 1$ and define \mathcal{Q}^d as $\{\vec{q}^d \in [0,1]^d : Pr[\max_{i=1}^{n(d)} ||\vec{q}^d - \vec{Y}_i||_p - (1 + \epsilon) \min_{i=1}^{n(d)} ||\vec{q}^d - \vec{Y}_i||_p \ge 0] \ge 1 - \zeta\}$ and $\mathcal{Q} = \prod_{d=1}^{\infty} \mathcal{Q}^d$. Clearly, for any $\{\vec{q}^d\} \in \mathcal{Q}$, $\lim_{d \to \infty} P_{d,n(\cdot),\vec{q}^d} \le \zeta$. Hence, all that remains is to show that \mathcal{Q} is large, *i.e.* for any $0 \le \omega < 1$, $\lim_{d \to \infty} \frac{Volume([0,\omega]^d)}{Volume(\mathcal{Q}^d)} = 0$.

Let \vec{Y} be distributed as f_d and be independent of $\vec{Y}_1, \ldots, \vec{Y}_{n(d)}$. Define random variables $D_{min} = \min_{i=1}^{n(d)} \{||\vec{Y} - \vec{Y}_i||_p\}$, $D_{max} = \max_{i=1}^{n(d)} \{||\vec{Y} - \vec{Y}_i||_p\}$. Such random variables (or related ones) have received considerable study in the stochastic geometry literature. Using one such study [9], we prove, in Appendix A, the following two inequalities with Z denoting $D_{max} - (1 + \epsilon)D_{min}$:

$$\lim_{d\to\infty} \frac{E[Z]}{d^{1/p}} \ge \frac{1}{100} \text{ and } Volume(\mathcal{Q}^d) \ge \left[\frac{1}{\zeta\beta(d)}\right] \left[\frac{E[Z]}{d^{1/p}} + \zeta - 1\right].$$
 (2)

For any $0 \le \omega < 1$, inequalities (2) as well as the assumptions that $99/100 < \zeta < 1$ and $\beta(d)$ grows sub-exponentially imply that $\lim_{d\to\infty} \frac{Volume([0,\omega]^d)}{Volume(\mathcal{Q}^d)} = 0$, as needed.

4. Multi-Variate Gaussian Distributions – Preliminary Results

We provide preliminary results concerning instability admission over an important class of distributions that do not satisfy our assumptions above: $\{N(\vec{\mu}_d, \Sigma_d)\}$. The following simple strategy yields a sufficient condition in the case that: $\vec{q}^d = 0$, $\vec{\mu}_d = 0$, p = 2, and the number of eigenvalues of Σ_d which do not go to zero grows faster than n(.). Using the eigenvalue decomposition of Σ_d , it can be shown that

$$\begin{split} & Pr\left[\left|||\vec{Y}_{1}||_{2}^{2} - E[||\vec{Y}_{1}||_{2}^{2}]\right| > E[||\vec{Y}_{1}||_{2}^{2}]\delta(\epsilon,2)\right] \\ = & Pr\left[\left|\sum_{j=1}^{d}W_{j}^{2} - E\left[\sum_{j=1}^{d}W_{j}^{2}\right]\right| > E\left[\sum_{j=1}^{d}W_{j}^{2}\right]\delta(\epsilon,2)\right], \end{split}$$

where the W's are independent and distributed as $N(0, \lambda_j^2)$ with λ_j the j^{th} largest eigenvalue of Σ_d . Chebyshev's inequality shows that the r.h.s. of the equation above is bounded above by

$$\left[\frac{2}{\delta(\epsilon,2)}\right] \left[\frac{\sum_{j=1}^{d} \lambda_j^4}{\sum_{i=1}^{d} \lambda_i^4 + 2\sum_{1 \le \ell \ne k \le d} \lambda_\ell^2 \lambda_k^2}\right].$$

Plugging this bound into the r.h.s. of inequality (1), with $\gamma = E[||\vec{Y}_1||_2^2]$, our assumptions above on n(.) and the $\lambda's$ imply that $\lim_{d\to\infty} P_{d,n(.),\vec{q}^d} = 1$.

Extending the above strategy to \vec{q}^d , $\vec{\mu}_d \neq 0$ and larger growth rates for n(.) seems possible utilizing more complex properties of weighted, non-central chi-square distributions. However, extending beyond p=2 seems difficult as only the 2-norm is preserved by orthogonal transformations. Also, extending beyond multi-variate Gaussian data distributions seems difficult owing to the fact that independence of the W's depends upon the Gaussian assumption.

A. Appendix: Some Proofs

First we prove the left inequality in (2): $\lim_{d\to\infty} \frac{E[Z]}{d^{1/p}} \ge \frac{1}{100}$, where $Z = D_{max} - (1 + \epsilon)D_{min} = \max_{i=1}^{n(d)} \{||\vec{Y} - \vec{Y}_i||_p\} - (1 + \epsilon)\min_{i=1}^{n(d)} \{||\vec{Y} - \vec{Y}_i||_p\}.$

Theorems 1.1 and 1.2 of [9] produce an upper-bound on $E[D_{min}]$ and a lower-bound on $E[D_{max}]$, respectively. These combine to yield⁵

$$\begin{split} \frac{E[Z]}{d^{1/p}} & \geq & \frac{\Gamma(n(d)+1/d)\Gamma(n(d)+1)}{d^{1/p}\Gamma(n(d))\Gamma(n(d)+1+1/d)3^{1/2}2^{1/d}e^{(1/2d)}||f_d||_2^{2/d}V_{d,p}^{1/d}} \\ & - & \frac{2(1+\epsilon)}{d^{1/p}(n(d)+1)^{1/d}V_{d,p}^{1/d}} - o\left(\frac{1+\epsilon}{d^{1/p}(n(d)+1)^{1/d}}\right). \end{split}$$

Thus,6

$$lim_{d\to\infty}\frac{E[Z]}{d^{1/p}} \geq lim_{d\to\infty}\left(\frac{1}{3^{1/2}d^{1/p}V_{d,p}^{1/d}} - \frac{1}{2d^{1/p}V_{d,p}^{1/d}}\right).$$

From [8] (using the fact that $p \ge 1$) and Stirling's approximation⁷ of Γ (.) (6.1.3.7 in [1]), $\lim_{d\to\infty} d^{1/p} V_{d,p}^{1/d} \le 2(ep)^{1/p}$. Hence, the above limit is bounded below by (1/100), as desired.

 $^{{}^5}V_{d,p}$ denotes the volume of the unit-ball in \mathbb{R}^d with respect to the *p*-norm. $\Gamma(.)$ denotes the standard gamma function.

 $^{^6}lim_{d\to\infty}||f_d||_2^{2/d} \le 1$ since $support(f_d) = [0,1]^d$ and sequence $\{f_d\}$ is bounded above sub-exponentially. Also, the ratio of the $\Gamma()'s$ approaches one because of the equality $\Gamma(z+1) = z\Gamma(z)$ for any $z \in \mathbb{R}$. Finally, $lim_{d\to\infty}(n(d)+1)^{1/d} \ge 4(1+\epsilon)$ since, by assumption, $n(d) > [4(1+\epsilon)]^d$ for large d.

⁷For large z, $\Gamma(z) \approx exp(-z)z^{z-1/2}(2\pi)^{1/2}$.

Now we prove the right inequality in (2): $Volume(\mathcal{Q}^d) \geq \left[\frac{1}{\zeta\beta(d)}\right] \left[\frac{E[Z]}{d^{1/p}} + \zeta - 1\right]$, where $\mathcal{Q}^d = \{\vec{q}^d \in [0,1]^d : Pr[\max_{i=1}^{n(d)} ||\vec{q}^d - \vec{Y}_i||_p - (1+\epsilon) \min_{i=1}^{n(d)} ||\vec{q}^d - \vec{Y}_i||_p \geq 0] \geq 1-\zeta\}$ and $99/100 < \zeta < 1$.

Let f_Z and $f_{Z|\vec{Y}}$ denote the p.d.f of Z and the conditional p.d.f of Z given \vec{Y} , respectively. Since $support(f_d) = [0,1]^d$, then $support(f_Z) \subseteq [0,d^{1/p}]$, thus, $E[Z] = \int_{z=0}^{d^{1/p}} z f_Z(z) \partial z \leq d^{1/p} \int_{z=0}^{d^{1/p}} f_Z(z) \partial z = d^{1/p} \int_{z=0}^{d^{1/p}} \int_{\vec{q}^d \in [0,1]^d} f_{Z|\vec{Y}}(z|\vec{q}^d) f_d(\vec{q}^d) \partial \vec{q}^d \partial z = d^{1/p} \int_{\vec{q}^d \in [0,1]^d} \int_{z=0}^{d^{1/p}} f_{Z|\vec{Y}}(z|\vec{q}^d) f_d(\vec{q}^d) \partial z \partial \vec{q}^d$. Hence,

$$\begin{split} \frac{E[Z]}{d^{1/p}} & \leq \int_{\vec{q}^d \in [0,1]^d} f_d(\vec{q}^d) \left[\int_{z=0}^{d^{1/p}} f_{Z|\vec{Y}}(z|\vec{q}^d) \partial z \right] \partial \vec{q}^d \\ & = \int_{\vec{q}^d \in [0,1]^d} f_d(\vec{q}^d) Pr \left[\max_{i=1}^{n(d)} \{||\vec{q}^d - \vec{Y}_i||_p\} - (1+\epsilon) \min_{i=1}^{n(d)} \{||\vec{q}^d - \vec{Y}_i||_p\} \geq 0 \right] \partial \vec{q}^d \\ & = \int_{\vec{q}^d \in \mathcal{Q}^d} f_d(\vec{q}^d) Pr \left[\cdots \right] \partial \vec{q}^d + \int_{\vec{q}^d \in ([0,1]^d \setminus \mathcal{Q}^d)} f_d(\vec{q}^d) Pr \left[\cdots \right] \partial \vec{q}^d \\ & \leq \int_{\vec{q}^d \in \mathcal{Q}^d} f_d(\vec{q}^d) \partial \vec{q}^d + (1-\zeta) \int_{\vec{q}^d \in ([0,1]^d \setminus \mathcal{Q}^d)} f_d(\vec{q}^d) \partial \vec{q}^d \\ & = Pr [\vec{Y} \in \mathcal{Q}^d] + (1-\zeta) Pr [\vec{Y} \in ([0,1]^d \setminus \mathcal{Q}^d)] \\ & = \zeta Pr [\vec{Y} \in \mathcal{Q}^d] + 1 - \zeta \\ & \leq \zeta \beta(d) Volume(\mathcal{Q}^d) + 1 - \zeta. \end{split}$$

The second inequality follows from the definition of Q^d and the last inequality follow from the assumption that f_d is bounded above sub-exponentially. The desired inequality follows.

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