Abstract

This paper discusses a new family of bounds for use in similarity search, related to those used in metric indexing, but based on Ptolemy’s inequality, rather than the metric axioms. Ptolemy’s inequality holds for the well-known Euclidean distance, but is also shown here to hold for quadratic form metrics in general. In addition, the square root of any metric is Ptolemaic, which means that the principles introduced in this paper have a very wide applicability. The inequality is examined empirically on both synthetic and real-world data sets and is also found to hold approximately, with a very low degree of error, for important distances such as the angular pseudometric and several $L_p$ norms. Indexing experiments are performed on several data sets, demonstrating a highly increased filtering power when using certain forms of Ptolemaic filtering, compared to existing, triangular methods. It is also shown that combining the Ptolemaic and triangular filtering can lead to better results than using either approach on its own.

Key words: Algorithms, Data Structures, Information Retrieval, Metric Indexing, Similarity Retrieval, Ptolemy’s Inequality

1. Introduction

In similarity search, data objects are retrieved based on their similarity to a query object; as for other modes of information retrieval, the related indexing methods seek to improve the efficiency the search. Two approaches seem to dominate the field: Spatial access methods [1–3], based on coordinate geometry, and metric access methods [4–7], based on the metric axioms. Similarity retrieval with spatial access methods is often restricted to $L_p$ norms, or other norms with predictable behavior in $\mathbb{R}^k$, while metric access methods are designed to work with a broader class of distances—basically any distance that satisfies the triangular inequality. This gives the metric approach a wider field of application, by foregoing some assumptions about the data, in some cases resulting in lower performance. Interestingly, even in cases where spatial access methods are applicable, metric indexing may be superior in dealing with high-dimensional data, because of its ability to bypass the so-called representational dimensionality and deal with the intrinsic dimensionality of the data directly [see, e.g., 8].

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It seems clear that there are advantages both to making strong assumptions about the data, as in the spatial approach, and in working directly with the distances, as in the metric approach. The direction taken in this paper is to apply a new set of restrictions to the distance, separate from the metric axioms, still without making any kind of coordinate-based assumptions. The method that is introduced is shown to hold a potential for highly increased filtering power, and while it holds for the square root for any metric, it is also shown analytically to apply to quadratic form metrics in general (with Euclidean distance as an important special case), and empirically, as an approximation with a very low degree of error, to important cases such as the angular pseudometric, edit distance between strings, and several $L_p$ norms.

2. Basic Concepts

The similarity in similarity retrieval is usually formalized, inversely, using a dissimilarity function, a nonnegative real-valued function $d(\cdot, \cdot)$ over some universe of objects, $U$. For typographic convenience, I will usually abbreviate $d(x, y)$ to $xy$, for all $x, y \in U$. A distance query consists of a query object $q$, and some form of distance threshold, either given as a range (radius) $r$, or as a neighbor count $k$. For the range query, all objects $o$ for which $qo \leq r$ are returned; for the $k$-nearest-neighbor query ($k$NN), the $k$ nearest neighbors of $q$ are returned, breaking ties arbitrarily. The $k$NN queries can be implemented in terms of range queries in a quite general manner [5].

For a function to qualify as a dissimilarity function (or premetric) the value of $xx$ must be zero. It is generally assumed (mainly for convenience) that the dissimilarity is symmetric ($xy = yx$, giving us a distance) and isolating ($xy = 0 \iff x = y$, yielding a semimetric). From a metric indexing perspective, it is most crucial that the distance be subadditive, or triangular (obeying the triangular inequality, $xz \leq xy + yz$). A metric is any symmetric, isolating, triangular dissimilarity function. Metrics are related to the concept of norms: A norm metric is a metric of the form $xy = \|x - y\|$, where $x$ and $y$ are vectors and $\|\cdot\|$ is a norm.

Many distances satisfy the metric properties (including several important distances over sets, strings and vectors), and metric indexing is the main approach in distance based (as opposed to coordinate based) retrieval. The metricity (triangularity, first and foremost) is exploited to construct lower bounds for efficient filtering and partitioning. As discussed in an earlier tutorial [7], there are several ways of using the triangular inequality in metric indexing, usually by pre-computing the distances between certain sample objects (called pivots or centers, depending on their use) and the other objects in the data set. By computing the distances between the query and the same sample objects (or some of them), triangularity can be used to filter out objects that clearly do not satisfy the criteria of the query.

Even though most distance based indexing has focused on the metric axioms, this paper focuses on another property, known as Ptolemy’s inequality, which entails that

$$xv \cdot yu \leq xy \cdot uv + xu \cdot yv,$$

for all objects $x, y, u, v$. Premetrics satisfying this inequality are called Ptole-
maic. In the terms of the Euclidean plane: For any quadrilateral, the sum of the pairwise products of opposing sides is greater than or equal to the product of the diagonals (see Fig. 1).

It is a well-known fact that Euclidean distance is Ptolemaic [10]. What is perhaps less well known is that there is a natural connection between Ptolemaic metrics on vector spaces and a generalization of Euclidean distance—a family of distances collectively referred to as quadratic form distance. A quadratic form distance may be expressed like this:

\[ d(x, y) = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} (x_i - y_i)(x_j - y_j)}, \]

or, in matrix notation, \( \sqrt{z^T A z} \), where \( x \) and \( y \) are vectors, and \( z = x - y \). The weight matrix \( A \) is a measure of “unrelatedness” between the dimensions, which uniquely defines the distance. We can, without loss of generality, assume that \( A \) is symmetric, as any antisymmetries will have no bearing on the distance [11]. In order for the distance to be a metric, \( A \) must also be positive-definite.\(^2\)

Quadratic form distances take into account possible correlations between the dimensions of the vector space, which make them especially suited for comparing histograms [see, e.g., 12]. For example, when comparing color histograms, it might be natural to compare the bin (that is, dimension) for orange to those of red and yellow [11]. If \( A \) is restricted to a diagonal matrix, a weighted Euclidean distance results, with the identity matrix leading to ordinary Euclidean distance (see Fig. 2). The fact that this important family of distances is usable with the techniques presented in this paper is expressed in the following theorem.

**Theorem 1.** A distance function is a quadratic form metric if and only if it is a Ptolemaic norm metric.

\(^1\)Note that Ptolemy’s inequality neither implies nor is implied by triangularity [9].

\(^2\)Some sources require only positive-semidefiniteness [e.g., 6], but this would result in a pseudometric, allowing a distance of zero between different objects. It is possible to relax the requirement on \( A \) by adding requirements to the inputs [11].
Proof. Let the quadratic form metric \( d(x, y) \) be \( \sqrt{z'Az} \), where \( z = x - y \). Because \( A \) is symmetric positive-definite, \( z'Az \) defines an inner product, making any such \( d \) a norm metric based on an inner product norm (a norm of the form \( \|z\| = \sqrt{\langle z, z \rangle} \), where \( \langle \cdot, \cdot \rangle \) is an inner product). Note that the converse also holds: Any inner product norm can be expressed as a quadratic form metric (with a positive-definite \( A \)). It is known that a norm metric is Ptolemaic if and only if its norm is an inner product norm \([10, 13]\), which gives us the theorem.

Beyond this, there are certainly many other Ptolemaic metrics (with the discrete metric, \( d(x, y) = 1 \Leftrightarrow x \neq y \), as an obvious example). In fact, for any metric \( d \), the metric \( \sqrt{d} \) is Ptolemaic \([14]\). In terms of distance orderings, and therefore similarity queries, this new metric is equivalent to the original, meaning that the techniques in this paper are applicable to all metrics. However, the transform will increase its intrinsic dimensionality \([15]\), making the process of indexing harder. As shown in Sect. 6.2, several non-Ptolemaic metrics seem to be “sufficiently Ptolemaic” to be used with the Ptolemaic indexing techniques without such a transform.

3. Related Work

As discussed at length elsewhere \([3\text{–}7]\), there are many published methods that deal with indexing distances based on the metric properties. While there has been an increasing focus on reducing I/O and general CPU time, the primary aim of most publications has been minimizing the number of distance computations, based on the assumption that the distance is highly expensive to compute.\(^3\) While focusing exclusively on this one performance criterion may not be altogether realistic (yielding, for example, methods with linear query time \([17, 18]\) or quadratic memory use \([19, 20]\)), it has proved a useful foundation on which methods with more nuanced performance properties could be

\(^3\)This assumption may very well stem from the seminal work of Feustel and Shapiro \([16]\), where calculation of the metric involved comparing every permutations of the node sets of two graphs.
This paper also focuses on minimizing distance computations, setting aside related questions of algorithm engineering for later.

The main mechanism through which distance calculations may be avoided is through various forms of filtering or exclusion, using lower bounds [7]. If the structure of the data objects is known, very precise, yet cheap, lower bounds can be constructed [25], but for metric indexing, only the general properties of the distance may be used. As described in Sect. 2, this is done by storing precomputed distances, or ranges of distances, involving the data set and certain sample objects (centers or pivots).

Rather than listing existing indexing methods, only the most relevant of the basic principles will be addressed here. Two rather general theorems contain the majority of the indexing principles as special cases. The first of these, dealing with metric balls, is given here without proof. The second, dealing with generalized hyperplanes, as well as more details and proofs for both theorems can be found in the aforementioned tutorial, the survey by Hjaltason and Samet [5] or the textbook by Zezula et al. [6]. In the following, let \( o, p \) and \( q \) be objects in a universe \( U \), and let the implicit distance \( d \) be a metric over \( U \).

**Theorem 2.** The value of \( qo \) may be bounded as

\[
\max\{\lfloor op \rfloor - \lceil qp \rceil, \lceil qp \rceil - \lfloor op \rfloor\} \leq qo \leq \lceil qp \rceil + \lceil op \rceil,
\]

where \( [uv] \leq uv \leq [uv] \), for any objects \( u, v \) in \( U \).

The expressions \( [uv] \) and \( [uv] \) refer to known lower and upper bounds for \( uv \), as, in some cases, these distances may not be fully known. For example, \( p \) may be the center of a metric ball containing \( o \), with covering radius \( r \). In that case \( [po] = 0 \) and \( [po] = r \). If the query–pivot distance is known, we get the lower bound

\[
qp - r \leq qo,
\]

which is exactly the bound used to check for overlap between a query ball and a bounding ball in a metric tree, for example.

4. Ptolemaic Pivot Filtering

In a manner similar to Theorem 2, Ptolemy’s inequality may be used to construct lower bounds for filtering. In the following, the technique known as pivoting is used. The derivation of a more general bound is deferred to Sect. 5.

Triangular pivoting is based on the following lower bound, a special case of the one in Theorem 2, where the distances are known exactly:

\[
qo \geq \lvert qp - op \rvert
\]

Here, \( q \) is the query object, \( o \) is a candidate result object, while \( p \) is a so-called pivot object, whose function is to help construct the bound.

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4The converse, inclusion using upper bounds, is also possible, but less frequently useful, simply because most of the data should normally be excluded from the result set.

5In the case of generalized hyperplane indexing, the information stored is simply which center is closest to a given object.
This bound follows from basic restructuring of the triangular inequality:

\[
op + qo \geq qp \\
qo \geq qp - op,
\]

and, in the same manner,

\[
qo \geq op - qp.
\]

Together, (4) and (5) lead directly to (3). The bound is normally strengthened by using a set of several pivots, \(P\):

\[
qo \geq \max_{p \in P} |qp - op|
\]

A similar derivation can be made for Ptolemaic metrics. In the following, \(q\), \(p\), and \(o\) retain their previous meaning, but we also add another pivot object, \(s\):

\[
qs \cdot op + qo \cdot ps \geq qp \cdot os \\
qo \cdot ps \geq qp \cdot os - qs \cdot op \\
qo \geq (qp \cdot os - qs \cdot op)/ps
\]

Here we can maximize over all pairs of pivots:

\[
qo \geq \max_{p,s \in P} \frac{qp \cdot os - qs \cdot op}{ps}
\]

By exchanging \(p\) and \(s\) in (6), we could exchange the terms in the numerator, allowing us to use the absolute value in (7). This would not strengthen the bound as it stands, but would allow us halve the number of pivot pairs examined.

For the normal pivoting bound to be useful, the pivot should closer to either the query or to the candidate object; the difference in the two distances is what gives the bound its filtering power. For the Ptolemaic pivoting bound, it seems that one way of getting good results would be to have one pivot close to the query, while the other is close to the candidate object, giving a high value for the numerator in (7). However, this intuition is tempered by the denominator, which dictates that the pivots should also be close to each other. Invariably, the tradeoff here will need to be based on empirical considerations.

As long as the distance matrix between the pivots is precomputed, the bound can be computed for every pair of pivots, and the maximum used as the final bound. As will be shown in Sect. 6, this Ptolemaic pivoting bound is a significant improvement over the classical triangular one.

The difference between triangular and Ptolemaic pivoting in the Euclidean plane is illustrated in Fig. 3, where the ratio between bound and distance from a query at \((-1,0)\), with the pivots placed at \((0,0)\) and \((1,0)\), is plotted for each point, where zero (a non-informative lower bound) is black and one (a perfect bound) is white.

While the the bound in (7) is the one examined in depth in this paper, the ideas of Ptolemaic indexing have wider implications. In the following section, a more general theorem (Theorem 3) is given, which is a Ptolemaic analogue of Theorem 2.
5. Generalizing the Ptolemaic Bound

The following theorem generalizes the bound (7), as a Ptolemaic analogue of Theorem 2. This generalization is included as a starting point for new indexing methods, and is not examined empirically in this paper.

**Theorem 3.** Let $o$, $p$, $q$ and $s$ be objects in a universe $U$, and let $d$ be a Ptolemaic distance over $U$. The value of $q_o$ may then be bounded as

$$
\frac{1}{|ps|} \cdot \max \left\{ \frac{|qs|}{|qp|} \cdot \frac{|os|}{|qp|} - \frac{|qp|}{|qs|} \cdot \frac{|os|}{|op|}, \frac{|qs|}{|qp|} \cdot \frac{|op|}{|qs|} - \frac{|qp|}{|os|} \cdot \frac{|op|}{|op|} \right\} \leq q_o \leq \frac{1}{|ps|} \cdot \left( \frac{|qp|}{|qs|} + \frac{|qs|}{|os|} \right),
$$

where $|uv| \leq uv \leq [uv]$, for any objects $u, v$ in $U$.

**Proof.** The two cases of the lower bound correspond to the two possible orderings of the products in the numerator of the lower bound (7), both of which are permissible. The only change here is that instead of the exact values, we use upper and lower limits. The lower limits occur before the subtractions, while the upper limits occur after, as well as in the denominator. These substitutions can only lower the value of the bound, and hence the inequality still holds. The upper bound follows from the Ptolemaic inequality

$$
ps \cdot qo \leq qp \cdot os + qs \cdot op.
$$

Dividing by $ps$ and safely substituting upper limits in the numerator and a lower limit in the denominator, we arrive at the upper bound.

The applications of this theorem to pivot filtering have already been discussed in Sect. 4. However, its metric analog, Theorem 2, is also used for

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6Note that $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ are not used to represent floor and ceiling here.
overlap checking with balls and shells, which is what the upper and lower limits to the distances represent. The notion of overlapping metric balls is inherently triangular, and does not directly translate to Ptolemaic distances. We are still able to exploit similar information, but we are in the somewhat unusual situation of working with two balls (or shells) at once. Take the upper bound, in the case where we know \( q_p \) and \( q_s \) (and, of course, \( p_s \)). In order to apply this bound (for automatic inclusion of \( o \)), we would have to know that \( o \) falls inside two balls, one around \( p \) and one around \( s \), with radii \( \lceil o_p \rceil \) and \( \lceil o_s \rceil \), respectively.

While this sort of “double containment” is not the norm in current metric indexing methods, it is certainly not impossible to implement. One would simply need to let each region be represented by two distance balls, and maintain two covering radii—one for each center. There is an inherent tradeoff here: If the objects are far apart, the covering radii will necessarily become quite large; however, if we move them closer, the upper bound will increase.

In considering the lower bound, we see something interesting: If we envision a structure with covering radii around both \( p \) and \( s \), the lower limits \( \lfloor o_p \rfloor \) and \( \lfloor o_s \rfloor \) both become zero, leaving us also with a total lower bound of zero. We see that, as for the pivot filtering case, we may need for one of the pivots to be more “query-like,” and the pivots need to be different from each other. For example, if the query is close to \( p \) but far from \( s \), and the converse holds for the object, the lower bound will be high. However, this may not be enough. Consider the case where the object falls within a ball with radius \( r \) around \( p \) (giving us \( \lfloor o_s \rfloor = p_s - r \)); we then get the following variation of the lower bound from (2):

\[
q_o \geq \frac{1}{p_s} \cdot (q_p \cdot (p_s - r) - r \cdot q_s) = q_p - r \cdot \frac{q_p + q_s}{p_s}
\]

The only difference from the triangular condition is the scaling factor \((q_p + q_s)/p_s\), which we can see as regulating the influence of the radius. If the query lies directly between \( p \) and \( s \) (that is, \( p_s = q_p + q_s \)) this new bound is, in fact, exactly equivalent to the triangular one. However, for all other cases, the new bound is worse.

What’s missing is the “other half,” as it were: an inverted ball around \( s \), excluding \( o \), giving us a proper \( \lceil o_s \rceil \), in addition to the covering radius, \( \lceil o_p \rceil \). This would be available in a situation where we have covering shells from each pivot to its sibling regions (as in GnAT [26] and its descendants), or where we use “inside/outside” partitioning with multiple pivots simultaneously (as in D-Index [27]). In such cases, where both upper and lower bounds are available for both \( q_p \) and \( o_s \), the bound in Theorem 3 can be used directly, substituting exact values for \( p_s, q_s \) and \( q_p \).

6. Experimental Results

Two sets of experiments have been performed to evaluate the usefulness of Ptolemy’s inequality in distance indexing: The first set of experiments evaluate its filtering power (using pivot filtering), while the second evaluates its recall rates for non-Ptolemaic metrics, for uses in approximate search.

6.1. Filtering Power for Ptolemaic Metrics

The first set of experiments were designed to compare the filtering power of the Ptolemaic and triangular approaches. Fig. 4 shows the results for pivot
filtering, with both the triangular and Ptolemaic lower bounds.

The first four data sets used were five- and ten-dimensional vectors. Both in five and ten dimensions, one uniformly random and one clustered data set were used. In the clustered case, vectors were drawn in equal proportion from ten gaussian clusters (with $\sigma^2 = 0.1$), centered around vectors drawn uniformly random from the unit hypercube. This clustering approach is similar to that used by Zezula et al. [21]. In addition, a set of 64-dimensional image histograms under a quadratic form distance was used, as well as another set of uniformly random ten-dimensional vectors, under the angular pseudometric (the angle formed by the vectors and the origin, also known as normalized correlation), which is equivalent, in terms of retrieval results, to the well-known cosine distance. The histogram distance used was similar to that described by Hafner et al. [11], using Euclidean distance in RGB space as the basis for the weight matrix. The histograms themselves were constructed by posterizing random images from an online image repository [28]. In all cases, the number of objects was 10,000. The pivot filtering was performed directly on a precomputed distance table, somewhat like in laesa [17]. In addition to the full Ptolemaic pivot filtering described in Sect. 4, a version was used that included each pivot only once, resulting in the bound being computed on $n - 1$ pairs (equivalent to $2n - 2$ bounds of the form of (7), because the absolute value was used), which gives a CPU use closer to that of traditional pivoting. Of course, there is a range of settings available here, from a linear number of bounds, to the quadratic number used by the full filter.

The pivots used were selected using the method of Pedreira and Brisaboa [18], which has the advantage of adapting the number of pivots automatically to the complexity of the data set. Note that this method has been designed to select pivots suitable for metric indexing, and may therefore be less suited to Ptolemaic methods.

The plots in Fig. 4 show the total number distance computations needed (that is, the number of pivots plus the number of candidate objects that must be explicitly examined using the actual distance function). The search radius (the horizontal axis) is described using the number of objects it encompasses (10–50). In each case, $m$ is the number of pivots used. The experiments were averaged over ten randomly generated data sets, each tested with 100 queries randomly drawn from the data set. As can be seen, for these cases, the full Ptolemaic approach clearly outperforms the triangular—especially for higher dimensionalities. The partial Ptolemaic filtering also offers significant advantages in several cases.

Note that the last experiment is approximate: The angular pseudometric is not Ptolemaic. Even so, the number of false negatives (indicated by the numbers next to each point on the graph) is fairly low, especially for the partial Ptolemaic filter. The suitability of such approximations for various other distances is explored further in Sect. 6.2. It is worth noting that the Ptolemaic filters used in Fig. 4 are pure, that is, not combined with a triangular bound. Fig. 5 illustrates

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7 The matrix used was $a_{ij} = 1 - d_{ij}/d_{\text{max}}$, where $i$ and $j$ are histogram bins.
8 For the color histograms, the data sets were identical.
9 The pivot objects were specifically excluded from being used as queries, as that would automatically have given all bounds optimal performance.
10 Note that uniform vectors have a higher intrinsic dimensionality than clustered vectors [4].
Figure 4: Distance computations for radii covering 10–50 neighbors (avg. over ten runs w/100 random queries; \(n = 10,000\)). Vectors were drawn randomly (with ten random Gaussian clusters, \(\sigma^2 = 0.1\), and uniformly) in five and ten dimensions. Except for the last two experiments (4(e) and 4(f)), which used a quadratic form distance and the angular pseudometric, the retrieval was performed in Euclidean space.
Figure 5: Relative filtering power of the triangular and Ptolemaic pivoting bounds for fixed-radius 10-NN queries on 10,000 uniformly random ten-dimensional vectors (100 queries, averaged over ten runs). The region marked “both” represents objects filtered out by both heuristics. All the gray regions represent true negatives, while the white region represents false positives, where actual distance computations are needed.

the relative contribution of the triangular and Ptolemaic pivoting bounds, if both are used in range search where the radius covers the ten nearest objects, on 100,000 uniformly random ten-dimensional vectors (averaged over ten data sets, each tested with 100 queries drawn randomly from the data set). The pivots were chosen uniformly at random from the data set. In this figure, only negatives are shown—that is, objects that need to be filtered out before the ten nearest neighbors are left. The four regions represent (1) objects filtered out only by the Ptolemaic bound, (2) objects that both bounds are able to filter out, (3) objects filtered out only by the triangular bound, and (4) objects that neither bound manages to disqualify.

It is clear that even for a relatively modest number of pivots, the filtering power of the Ptolemaic bound is high, and the difference in the exclusive contributions of the two bounds is surprisingly large. At ten pivots, the Ptolemaic bound filters out $93.0\%$.

A progression similar to that in Fig. 5 was also found for clustered data, with a somewhat less pronounced difference (data not shown).

6.2. Approximation Rates for Non-Ptolemaic Metrics

Although the proposed approach is strictly correct only for Ptolemaic distances, it might also work well as an approximation for other distances; Fig. 4(f) already gives some indication of this. While any metric can be made Ptolemaic, as mentioned in Sect. 2, the resulting metric may be harder to index, and approximate indexing of the original may still be useful. Table 1 shows results for several data sets and distances. The three types of objects used were vectors, sets and strings. The vectors were generated as described in Sect. 6.1. The sets were generated randomly for a given maximum cardinality by including or excluding each object with equal probability. The string data sets were a list of 234,936 words from Webster’s Second International Edition, as distributed with the Macintosh OS version 10.5, and the lines of A Tale of Two Cities by Charles Dickens.
Table 1: Results from approximation experiments. The values given are the average Ptolemaic proportions of the quadruples, as well as the standard deviations. Subscripts on numbers represent powers of ten. \( \mathbb{R}^k \) refers to vectors of dimension \( k \), while \( 2^k \) are sets of cardinality \( k \).

| Distance      | \( L_1 \) Manhattan distance | \( L_2 \) Euclidean distance* | \( L_3 \) | \( L_5 \) | \( L_{10} \) | \( L_{100} \) | \( L_\infty \) Chebyshev distance | \( \theta \) Angular distance |
|--------------|-------------------------------|-------------------------------|--------|--------|--------|--------|-------------------------------|--------------------------|
| \( \mu \)   | 0.98                          | 0.99                          | 0.97   | 0.96   | 0.96   | 0.96   | 0.96                          | 0.99                     |
| \( \sigma \) | 1.70\text{E}^{-3}            | 6.39\text{E}^{-4}            | 1.39\text{E}^{-3} | 1.41\text{E}^{-3} | 2.01\text{E}^{-3} | 5.78\text{E}^{-4} | 2.09\text{E}^{-3} | 5.78\text{E}^{-4} |
| \( \mu \)   | 1.00                          | 1.00                          | 1.00   | 1.00   | 1.00   | 1.00   | 1.00                          | 1.00                     |
| \( \sigma \) | 3.81\text{E}^{-4}            | 1.11\text{E}^{-4}            | 1.31\text{E}^{-3} | 6.03\text{E}^{-4} | 1.49\text{E}^{-3} | 1.19\text{E}^{-4} | 1.45\text{E}^{-3} | 1.19\text{E}^{-4} |

For the vector data sets, various \( L_p \) norms were used, as well as the angular pseudometric. For the sets, the related Hamming and Jaccard distances were used (the cardinality of the symmetric difference, and proportion of the symmetric difference to the union, respectively), while for the strings, Levenshtein distance (edit distance) was used.

Each experiment was averaged over ten runs. Except for the string data sets, which were static, new data sets were randomly generated for each run. A run consisted of 10,000 randomly sampled quadruples (that is, sets of four distinct objects), and the proportion of the quadruples that satisfied Ptolemy’s inequality was computed.

As can be seen from Table 1, the much-used \( L_p \) norms vary in their approximation rates from 99.

The set distances also seem to conform to Ptolemy’s inequality to a high degree for the 20-dimensional case, and the edit distance has a very low rate of inequality violations (with the Dickens data set outperforming the Webster data set by several orders of magnitude). For the \( L_p \) spaces and the angular pseudometric, the intrinsic dimensionality was generally close to the actual number of dimensions (slightly higher for uniformly random vectors, and varying with \( p \)). The dimensionalities for the Hamming spaces were equal to about half the set cardinalities, while those for Jaccard distance were about 50.
7. Discussion and Future Work

In summary, this paper has presented a new distance indexing principle, based on Ptolemy’s inequality, which seems to result in greatly increased filtering power, in the cases where it is applicable. For vector spaces (in particular, \( \mathbb{R}^k \)), it is directly applicable to quadratic form distances, including Euclidean distance. It is also applicable to the square root of any metric, and approximately applicable, with a very high degree accuracy, to other distances such as the angular pseudometric and edit distance over strings.

While the experiments performed in this paper have shown that the Ptolemaic approach has potential for improved filtering, and therefore performance, over the purely triangular approach, the surface has barely been scratched when it comes to describing the properties of the new bounds. In the following, two main avenues for future research are outlined.

- The performance studies in this paper have the traditional pure filtering focus, only counting distance computations. It would be useful to examine the performance of Ptolemaic indexing in a more realistic setting, where queries are timed on real-world data. As the full Ptolemaic pivoting is computationally more expensive than the triangular version (a quadratic versus linear cost in the number of pivots), there would be a tradeoff in terms of distance computation cost, pivoting cost and filtering power. The number of bounds actually computed, in the spectrum from linear to quadratic, would be an important optimization parameter here. It might even be feasible to heuristically look for high bounds to compute, by examining the distances involved. For real-time testing like this, it would also be relevant to compare the distance-based algorithms to spatial access methods [1, 2], where possible.

- It would be interesting to examine the basic properties of the Ptolemaic pivots, as related to the space (including which composition of pivots that would give the best pivoting results). It seems that higher dimensionalities give Ptolemaic indexing a greater edge over the triangular one. In the experiments performed here, this may be due to the increased number of pivots, but even the partial Ptolemaic filtering increases its lead with with higher dimension and a higher pivot number, which cannot be explained by the quadratic growth in the number of bounds. This is certainly an issue worthy of further examination. It also seems like high-dimensional spaces are more likely to be approximately Ptolemaic—perhaps because the distances are more similar. Based on this reasoning, high-dimensional spaces would also be more likely to be approximately triangular. Taking the square root, which will increase the intrinsic dimension, will make any metric exactly Ptolemaic. On the other hand, both the Ptolemaic and the triangular bound will be weaker in these cases, so there is clearly a tradeoff between accuracy and filtering power. These are issues that could be examined both empirically and analytically.

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