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Realizing Euclidean distance matrices by sphere intersection

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Abstract

This paper presents the theoretical properties of an algorithm to find a realization of a (full) $n \times n$ Euclidean distance matrix in the smallest possible embedding dimension. Our algorithm performs linearly in $n$, and quadratically in the minimum embedding dimension, which is an improvement w.r.t. other algorithms.

Keywords: Distance geometry, sphere intersection, euclidean distance matrix, embedding dimension.

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1. Introduction

Euclidean distance matrices and sphere intersection have a strong mathematical importance \cite{1 2 3 4 5 6}, in addition to many applications, such as navigation problems, molecular and nanostructure conformation, network localization, robotics, as well as other problems of distance geometry \cite{7 8 9}.

Before defining precisely the problem of interest, we need the formal definition for Euclidean distance matrices. Let $D$ be a $n \times n$ symmetric hollow (i.e., with zero diagonal) matrix with non-negative elements. We say that $D$ is a (squared) Euclidean Distance Matrix (EDM) if there are points $x_1, x_2, \ldots, x_n \in \mathbb{R}^K$ (for a positive integer $K$) such that

$$D(i,j) = D_{ij} = \|x_i - x_j\|^2, i,j \in \{1, \ldots, n\},$$

where $\|\cdot\|$ denotes the Euclidean norm. The smallest $K$ for which such a set of points exists is called the embedding dimension of $D$, denoted by $\dim(D)$. If $D$ is not an EDM, we define $\dim(D) = \infty$.

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We are concerned with the problem of determining $\dim(D)$ for a given symmetric hollow matrix $D$, which is known as the EDM recognition problem. If $\dim(D) = K < \infty$, we also want to determine a sequence $x = (x_1, \ldots, x_n)$ of $n$ points in $\mathbb{R}^K$ such that $D$ is the EDM of $x$ (this is called a realization of $D$). We emphasize that $D$ is a full matrix: this strikes a difference with much of the Distance Geometry literature, which is concerned with the problem of completing partial EDMs in a given embedding dimension [4].

The best known algorithm for solving the EDM recognition problem is classic Multidimensional Scaling (MDS) [10]. Given a symmetric hollow matrix $D$, compute $G = -\frac{1}{4}JDJ$ (where $J = I - \frac{1}{4}11^T$, $I$ is the identity matrix and $1$ is the all-one vector) and its spectral decomposition $G = P\Lambda P^t$, where $\Lambda = \text{diag}(\lambda)$ and $\lambda$ is the vector $\lambda = (\lambda_1, \ldots, \lambda_n)$ of eigenvalues of $G$ in decreasing order. If there is $i \leq n$ with $\lambda_i < 0$ then $D$ is not an EDM, otherwise it is. In this case a realization is given by $x = \sqrt{\Lambda}$, and the minimum embedding dimension is given by the index $K \leq n$ such that $\lambda_K$ is the smallest nonzero eigenvalue. Other methods (e.g. [11, 4]), appear to be variants of the idea behind MDS, which is actually due to Schoenberg [12]. Since it requires matrix decomposition, all these methods are $O(n^2)$ (with $2 < \omega < 2.376$) by [13], though the consensus seems to be that they are $O(n^3)$ “in practice”.

This paper presents the theoretical background of the algorithm proposed in [13], where it was just described and illustrated with computational results. This algorithm solves the EDM recognition problem in $O(n \dim(D)^2)$. Since usually EDMs correspond to fixed embedding dimensions, our algorithm could be regarded as $O(n)$.

2. A new EDM recognition algorithm

This section presents the theoretical basis for the algorithm. While some of the results leading up to our main Theorem 1 are part of the standard distance geometry and linear algebra literature, we list them to make our treatment self-contained. In particular, our main theorem depends on Lemmata 2, 3 in turn, Lemma 3 depends on Prop. 2 which depends on Lemma 1 which depends on Prop. 1.

Let $I_n = \{1, \ldots, n\}$ and $I_{n_1, n_2} = \{n_1, n_1 + 1, \ldots, n_2 - 1, n_2\}$. Furthermore, if $U, V \subseteq I_n$ such that $V = \{v_1, \ldots, v_{n_1}\}$, $U = \{u_1, \ldots, u_{n_2}\}$ and $D$ is an $n \times n$ matrix, then $D(V, U) = (d_{ij})$ is the submatrix of $D$ such that $d_{ij} = D(v_i, u_j)$ with $i \in I_{n_1}$ and $j \in I_{n_2}$. Given a positive integer $n$, we define $\{x_i\}_{i=1}^n = \{x_1, x_2, \ldots, x_{n-1}, x_n\}$.

The following is a well-known result that provides an upper bound on the embedding dimension of a given EDM as a function of its order.

**Proposition 1.** Let $D$ be a $n \times n$ EDM. Then $\dim(D) \leq n - 1$.

**Proof.** If $D$ is a $n \times n$ EDM, then exists $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^m$ for any $m \geq \dim(D)$ which realizes $D$. Let $k$ be the dimension of the linear subspace generated by the vectors $\{x_i - x_1\}_{i=2}^n \subseteq \mathbb{R}^m$. Since this space is a $k$-dimensional subspace.
of $\mathbb{R}^m$, then it is isomorphic to $\mathbb{R}^k$ by a linear isometry $Q$. Let $y_1 = 0$ and 
$\{y_i = y_1 + Q(x_i - x_1)\}_{i=1}^n$. Thus,
$$
\|y_i - y_j\| = \|y_1 + Q(x_i - x_1) - y_1 - Q(x_j - x_1)\| = \|Q(x_i - x_j)\| = \|x_i - x_j\|
$$
for all $i, j \in I_n$. From this, we have that $\{y_i\}_{i=1}^n \subseteq \mathbb{R}^k$ also realizes $D$. Therefore
$\dim(D) \leq k \leq n - 1$. □

In order to present our main result (Thm. 1), we need some preliminary results. Lemma 1 and Prop. 2 state the well known fact that two different realizations of an EDM are isometric.

**Lemma 1.** Let $D$ be a $n \times n$ EDM and $\{x_i\}_{i=1}^n, \{y_i\}_{i=1}^n \subseteq \mathbb{R}^m$, for any $m \geq \dim(D)$, sets of points which realize $D$. For $i, j, k \in I_n$, we have:
$$
(x_i - x_j)^t(x_k - x_j) = (y_i - y_j)^t(y_k - y_j).
$$

**Proof.** Without loss of generality, let us assume that $i < j < k$. Let $D'$ be the EDM realized by the subset of points $\{x_i, x_j, x_k\}$ and $\{y_i, y_j, y_k\}$. From Proposition 1 there exist $\bar{x}_i, \bar{x}_j, \bar{x}_k$, $\bar{y}_i, \bar{y}_j, \bar{y}_k \subseteq \mathbb{R}^2$ which realize $D'$. We notice that, by the isometry used in Proposition 1, $(\bar{x}_i - \bar{x}_j)^t(\bar{x}_z - \bar{x}_j)$ and $(\bar{y}_i - \bar{y}_j)^t(\bar{y}_z - \bar{y}_j) = (\bar{y}_i - \bar{y}_j)^t(\bar{y}_z - \bar{y}_j)$. Since
$$
\|\bar{x}_i - \bar{x}_j\| = \|\bar{y}_i - \bar{y}_j\|
$$
$$
\|\bar{x}_i - \bar{x}_k\| = \|\bar{y}_i - \bar{y}_k\|
$$
$$
\|\bar{x}_j - \bar{x}_k\| = \|\bar{y}_j - \bar{y}_k\|,
$$
we have that the triangles obtained are similar. Therefore,
$$
(\bar{x}_i - \bar{x}_j)^t(\bar{x}_k - \bar{x}_j) = (\bar{y}_i - \bar{y}_j)^t(\bar{y}_k - \bar{y}_j).
$$

Thus,
$$
(x_i - x_j)^t(x_k - x_j) = (\bar{x}_i - \bar{x}_j)^t(\bar{x}_k - \bar{x}_j) = (\bar{y}_i - \bar{y}_j)^t(\bar{y}_k - \bar{y}_j) = (y_i - y_j)^t(y_k - y_j).
$$

We say that two subsets of points $\{x_i\}_{i=1}^n, \{y_i\}_{i=1}^n \subseteq \mathbb{R}^m$ for any $m \geq \dim(D)$ are orthogonally similar if there is an orthogonal operator $Q$ on $\mathbb{R}^m$, such that $Q(x_i - x_j) = y_i - y_j$, for $i, j \in I_n$. We denote the subspace spanned by vectors $v_1, \ldots, v_n$ by $[v_i]_{i=1}^n$.

**Proposition 2.** Let $D$ be a $n \times n$ EDM and $\{x_i\}_{i=1}^n, \{y_i\}_{i=1}^n \subseteq \mathbb{R}^m$, for any $m \geq \dim(D)$, be sets of points which realize $D$. Then, $\{x_i\}_{i=1}^n$ is orthogonally similar to $\{y_i\}_{i=1}^n$. 

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Corollary 1. Let \( D \) be a \( n \times n \) EDM and \( \{x_i\}_{i=1}^n \subseteq \mathbb{R}^m \), for any \( m \geq \dim(D) \), a set of points which realizes \( D \). Then, the dimension of \( [x_i - x_1]_{i=2}^n \) is equal to \( \dim(D) \).

Lemmas 2 and 3 are new (as far as we know) and crucial for our main theorem. Given a EDM of order \( n \), the following result establishes that the embedding dimension of the given EDM is greater than the embedding dimension of any of its \( (n-1) \)-th principal submatrices by at most one. We denote by \( D(I_n, I_n) \) the \( n \)-th principal submatrix of \( D \).

Lemma 2. Let \( D \) be a \( (n+1) \times (n+1) \) EDM. If \( \dim(D(I_n, I_n)) = K \), then \( \dim(D) \in \{K, K+1\} \).

Proof. Let \( \{x_i\}_{i=1}^{n+1} \) be a set of points in \( \mathbb{R}^{K+1} \) that realizes \( D \) and the set of vectors \( \{v_i = x_i - x_1\}_{i=2}^{n+1} \). We have that \([v_i]_{i=2}^n \) is a linear \( K \)-dimensional subspace, since \( \{x_i\}_{i=1}^n \) realizes \( D(I_n, I_n) \) and \( \dim(D(I_n, I_n)) = K \). Therefore, we have

\[
\dim([v_i]_{i=2}^n) \leq \dim([v_i]_{i=2}^{n+1}) \leq \dim([v_i]_{i=2}^n) + \dim([v_i]_{i=n+1})
\]

\[
\Rightarrow \dim(D(I_n, I_n)) \leq \dim(D) \leq \dim(D(I_n, I_n)) + 1
\]

\[
\Rightarrow K \leq \dim(D) \leq K + 1.
\]
The next lemma ensures that, given a set \( S \subset \mathbb{R}^m \) of \( n \) points that realizes the \( n \)-th principal submatrix of a EDM of order \( n+1 \) with embedding dimension at most \( m \), \( S \) can be augmented into a realizing set for the full matrix without any change on the space dimension.

**Lemma 3.** Let \( D \) be a \((n+1) \times (n+1)\) EDM and \( \dim(D) \leq m \). Additionally, let \( \{x_i\}_{i=1}^n \subset \mathbb{R}^m \) be a set of points that realizes \( D(I_n, I_n) \). Then, there exists \( x_{n+1} \in \mathbb{R}^m \) such that \( \{x_i\}_{i=1}^{n+1} \) realizes \( D \).

**Proof.** Let \( \{y_i\}_{i=1}^{n+1} \subset \mathbb{R}^m \) be a set of points that realizes \( D \) and let \( \{x_i\}_{i=1}^n \) be a set of points that realizes \( D(I_n, I_n) \). By Proposition \( 2 \), we have that \( \{y_i\}_{i=1}^n \) and \( \{x_i\}_{i=1}^n \) are orthogonally similar, i.e., there is a linear operator \( Q \) on \( \mathbb{R}^n \) such that \( Q(y_i - y_j) = x_i - x_j \), for \( i, j \in I_n \). If \( x_{n+1} = x_1 + Q(y_{n+1} - y_1) \), then, for \( i \in I_n \),

\[
\|x_{n+1} - x_i\| = \|x_1 - x_i + Q(y_{n+1} - y_1)\| \\
= \|Q(y_1 - y_i) + Q(y_{n+1} - y_1)\| \\
= \|Q(y_1 - y_i + y_{n+1} - y_1)\| \\
= \|Q(y_{n+1} - y_1)\| \\
= \|y_{n+1} - y_1\|.
\]

Therefore, \( \{x_i\}_{i=1}^{n+1} \) realizes \( D \). \( \Box \)

The following theorem establishes necessary and sufficient conditions for a \( n \times n \) symmetric hollow matrix with nonnegative elements to be an EDM. If this matrix is a EDM with \( \dim(D) = K \), then there exists a set of points which realizes \( D \) such that \( K+1 \) of them form the columns of a triangular matrix.

**Theorem 1.** Let \( K \) be a positive integer and \( D \) be a \( n \times n \) symmetric hollow matrix with nonnegative elements, with \( n \geq 2 \). \( D \) is an EDM with \( \dim(D) = K \) if and only if there exist \( \{x_i\}_{i=1}^n \subset \mathbb{R}^K \) and an index set \( I = \{i_1, \ldots, i_{K+1}\} \subset I_n \) such that

\[
\begin{cases}
  x_{i_1} = 0 \\
  x_{i_j}(j - 1) \neq 0, & j \in I_{2,K+1} \\
  x_{i_j}(i) = 0, & j \in I_{2,K}, i \in I_{j,K},
\end{cases}
\]

where \( \{x_i\}_{i=1}^n \) realizes \( D \).

**Proof.** Let \( K \) be a positive integer and \( D \) be a \( n \times n \) EDM such that \( \dim(D) = K \). We want to show that there is a realization \( \{x_i\}_{i=1}^n \subset \mathbb{R}^K \) and an index set \( I = \{i_j\}_{j=1}^{K+1} \subset I_n \) with \( K+1 \) elements such that

\[
\begin{cases}
  x_{i_1} = 0 \\
  x_{i_j}(j - 1) \neq 0, & j \in I_{2,K+1} \\
  x_{i_j}(i) = 0, & j \in I_{2,K}, i \in I_{j,K},
\end{cases}
\]

where \( \{x_i\}_{i=1}^n \) realizes \( D \) (recall that \( x_{ij} \) is the \( j \)-th component of the vector \( x_i \)).
We remark that, since $K$ is a positive integer, then $D \neq 0$. We proceed by induction on $n$. For $n = 2$, we have

$$D = \begin{pmatrix} 0 & D(1,2) \\ D(1,2) & 0 \end{pmatrix}.$$ 

Therefore, $\dim(D) = 1$, $\{x_1 = 0, x_2 = \sqrt{D(1,2)}\} \subset \mathbb{R}^1$, $I = \{1,2\}$, and the statement is true.

As induction hypothesis, suppose that the statement is true for some $n \geq 2$. Let $D$ be a $(n+1) \times (n+1)$ EDM such that $\dim(D) = K$. Thus, $\bar{D} = D(I_n, I_n)$ is a EDM such that, by Lemma 2, $\dim(\bar{D}) = k$, with $k = K$ or $k = K - 1$.

From the induction hypothesis, there exist $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^k$ which realizes $\bar{D}$ and an index set $I = \{i_j\}_{j=1}^{k+1} \subseteq I_n$ with $k+1$ elements such that

$$\begin{cases}
    x_{i_1} = 0 \\
    x_{i_j}(j-1) \neq 0, & j \in I_{2,k+1} \\
    x_{i_j}(i) = 0, & j \in I_{2,k}, i \in I_{j,k}.
\end{cases}$$

Without loss of generality, we can assume $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^{k+1}$, by defining the $(k+1)$st coordinate of each vector to be zero. Since $\dim(D) \leq (k+1)$, by Lemma 3 there exists a vector $y = (y_1, y_2, \cdots, y_{k+1})$ in $\mathbb{R}^{k+1}$ such that $\{x_i\}_{i=1}^n \cup \{y\}$ realizes $D$.

This means that $y$ belongs to the intersection of the spheres centered in $\{x_i\}_{i=1}^n \subseteq \mathbb{R}^{k+1}$, each one with radius $\sqrt{D(i,n+1)}$. Therefore, $y$ is the solution of the following non-linear system:

$$\begin{cases}
    \|x_1 - y\|^2 = D(n,n+1) \\
    \|x_2 - y\|^2 = D(n,n+1) \\
    \vdots \\
    \|x_n - y\|^2 = D(n,n+1).
\end{cases}$$

Reordering the equations in such a way that the $j$-th equation is $\|x_{i_j} - y\|^2 = D(i,j,n+1)$, for $j \in I_{k+1}$, we have

$$\begin{cases}
    \|x_{i_1} - y\|^2 = D(i_1,n+1) \\
    \|x_{i_2} - y\|^2 = D(i_2,n+1) \\
    \vdots \\
    \|x_{i_{k+1}} - y\|^2 = D(i_{k+1},n+1) \\
    \|x_{j_1} - y\|^2 = D(j_1,n+1) \\
    \|x_{j_2} - y\|^2 = D(j_2,n+1) \\
    \vdots \\
    \|x_{j_{n-k-1}} - y\|^2 = D(j_{n-k-1},n+1),
\end{cases}$$

where $\{j_i\}_{i=1}^{n-k-1} = I_n \setminus I$. Applying the induction hypothesis, we know the points $\{x_{i_j}\}_{j=1}^{k+1}$. Using this information and subtracting the first equation from
the others, we obtain:

\[
\begin{align*}
\|y\|^2 &= D(i_1, n + 1) \\
x^T_{i_2} y &= b_{i_2} \\
\vdots \\
x^T_{i_{k+1}} y &= b_{i_{k+1}} \\
\vdots \\
x^T_{j_1} y &= b_{j_1} \\
x^T_{j_1} y &= b_{j_2} \\
x^T_{j_{n-k-1}} y &= b_{j_{n-k-1}},
\end{align*}
\]

where

\[b_i = \frac{\|x_i\|^2 - D(i, n + 1) + D(i_1, n + 1)}{2},\]

for \(i \in I_n \setminus \{i_1\}\). Let \(B\) be the \((n-1) \times k\) matrix associated with the linear part of the non-linear system and let \(b\) be the corresponding solution vector, both of them ordered according to the system above. Then, we can rewrite the system of equations as follows:

\[
\begin{align*}
\|y\|^2 &= \bar{D}(i_1, n + 1) \\
B y(I_k) &= Pb,
\end{align*}
\]

where \(P\) is a permutation matrix that defines the order used in the previous equations.

By construction, we have that \(B\) is a lower triangular matrix without null elements in the diagonal. Therefore, the linear part of the system has only two possible outcomes: a unique solution, or no solution. If the system has no solution, then the set generated by the intersection of the spheres in \(\mathbb{R}^{k+1}\) is empty, and thus, \(D\) is not a EDM, which is an absurd. Therefore, the linear part of the system has a unique solution \(y^*\).

Substituting this solution from the linear system into \(\|y\|^2 = \|y(I_k)\|^2 + y_{k+1}^2 = D(i_1, n + 1)\), we obtain

\[y_{k+1}^2 = D(i_1, n + 1) - \|y^*\|^2.\]

If \(D(i_1, n + 1) - \|y^*\|^2\) is negative, then the system has no solution, i.e., the intersection of the spheres in \(\mathbb{R}^{k+1}\) is empty, and thus, \(D\) is not a EDM. Again, an absurd. Therefore, the difference is not negative. If the difference is null, then \(K = k\) and the last entry of each point is unnecessary and the index set of the induction hypothesis remains valid and the statement is true.

If the difference is strictly positive, then \(k = K - 1\), implying the existence of two solutions, from which we must choose one (see Remark 3 in Sect. 2.1). If we define \(x_{n+1} = y\) and \(\tilde{I} = I \cup \{n+1\}\) as the index set, there exists \(\{x_i\}_{i=1}^{n+1} \subseteq \mathbb{R}^{k+1}\)
which realizes $D$ and an index set $\bar{I} = \{i_j\}_{j=1}^{K+1} \subseteq I_{n+1}$ with $K + 1$ elements, such that
\[
\begin{align*}
x_{i_1} &= 0 \\
x_{i_j}(j-1) &\neq 0, \quad j \in I_{2,K+1} \\
x_{i_j}(i) &= 0, \quad j \in I_{2,K}, i \in I_{j,K}.
\end{align*}
\]
This concludes the proof. \hfill $\square$

This induction process suggests an algorithm to verify whether or not a matrix $D$ is an EDM. If this is true, the algorithm also determines an embedding in the least possible dimension. The procedure is shown in Alg. 1 and we refer to it as edmsph, from “EDM” and “sphere”. The pseudocode makes use of a function expand$(x)$ which endows point vectors in the sequence $x$ with an additional zero component. We denote the sphere centered in $p \in \mathbb{R}^{K+1}$ with radius $r$ by $S^K(p,r)$.

\begin{algorithm}
K = edmsph(D,x)
1: $I = \{1,2\}$
2: $K = 1$
3: $(x_1,x_2) = (0,\sqrt{D_{12}})$
4: for $i \in \{3,\ldots,n\}$ do
5: $\Gamma = \bigcap_{j \in I} S^K(x_j,D_{ij})$
6: if $\Gamma = \emptyset$ then
7: return $\infty$
8: else if $\Gamma = \{p_i\}$ then
9: $x_i = p_i$
10: else if $\Gamma = \{p_i^+,p_i^-\}$ then
11: $x_i = p_i^+$
12: $x \leftarrow$ expand$(x)$
13: $I \leftarrow I \cup \{i\}$
14: $K \leftarrow K + 1$
15: else
16: error: dim aff(span$(x_I)) < K - 1$
17: end if
18: end for
19: return $K$
\end{algorithm}

2.1. Remarks

1. Given $K$ spheres in $\mathbb{R}^K$, we assume that their centers are in general position, i.e. they span a $(K-1)$-dimensional affine space. Then, we have at most two points in the intersection of these spheres. More specifically, we have no point if the intersection is empty, one point if the intersection lies in the $(K-1)$-dimensional affine space generated by the centers, and two points if there are no points in the intersection in the $(K-1)$-dimensional affine space generated by the centers. We also remark that
requiring general positions is sufficient to ensure the ensuing property but not necessary. At present, we still do not know how to weaken our general position requirements so that it is both necessary and sufficient to ensure that the number of points in the intersection of $K$ sphere is in $\{0, 1, 2\}$.

2. The error occurring in Line 16 of Alg. 1 is related to the remark above: if $\dim \text{aff}(\text{span}(x_I)) < K - 1$ the points in $x_I$ cannot be in general position in $\mathbb{R}^K$.

3. Note that $p_i^-$ is being ignored in Alg. 1 in fact its presence only serves the purpose of recognizing the need for increasing the current embedding dimension. The fact that we always just keep $p_i^+$ is arbitrary: other valid realizations would result from taking any combination of $+$ and $-$ alternatives. By [15 Lemma 4.3], $p_i^+, p_i^-$ are reflections of each other w.r.t. the hyperplane passing through preceding points $x_1, \ldots, x_k$ having affine dimension $k - 1$, the embedding dimension of $\{x_1, \ldots, x_{i-1}, p_i^+\}$.

Informally, every time the current embedding dimension is increased, there is the possibility of a new reflection acting on the partial realization found so far. If $\dim(D) = K$, then there will be $2^{K-1}$ realizations of $D$ modulo translations and rotations. Of course, there is only one realization modulo congruences (i.e. rotations, translations and reflections).

2.2. Complexity of Alg. 1

Using trilateration on the appropriately indexed points guaranteed by Thm. 1 finding $\Gamma$ in Alg. 1 requires solving a triangular linear system, which can be carried out in time proportional to $\bar{K}^2$. This leads to a total time of $O(n\bar{K}^2)$, where $\bar{K}$ is assumed to be a given upper bound to $K$ ($K$ is bounded below by the highest value taken by $K$ during the edmsph algorithm).

3. Conclusion

We presented the theoretical properties of a new algorithm which determines whether a given symmetric hollow (i.e., with zero diagonal) matrix with non-negative elements is a EDM. Additionally, if the matrix is indeed a EDM, the algorithm computes the matrix’s embedding dimension, alongside an actual embedding. This paper only addresses the case of exact distances; extensions to noisy or interval distances will be considered in subsequent works.

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