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An algorithm for realizing Euclidean distance matrices

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Abstract

We present an efficient algorithm to find a realization of a (full) $n \times n$ squared Euclidean distance matrix in the smallest possible dimension. Most existing algorithms work in a given dimension: most of these can be transformed to an algorithm to find the minimum dimension, but gain a logarithmic factor of n in their worst-case running time. Our algorithm performs cubically in n (and linearly when the dimension is fixed, which happens in most applications).

Keywords: Distance geometry, sphere interesection, EDM, embedding dimension.

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1 Introduction

The problem of adjustment of distances among points has been studied since the first decades of the 20th century [2]. It can be formally defined as follows: 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 $x_1, x_2, \ldots, x_n \in \mathbb{R}^K$, 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 $\mathsf{dim}(D)$. If D is not an EDM, we define $\mathsf{dim}(D) = \infty$.

We are concerned with the problem of determining $\mathsf{dim}(D)$ for a given symmetric hollow matrix D. If $\mathsf{dim}(D) = K < \infty$, 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. We emphasize that D is a full matrix.

In the literature we prevalently find efficient methods for solving a related problem, i.e. whenever K is given as part of the input (see e.g. [1,6,7]). Each of these algorithms can be used within a bisection search to determine the embedding dimension, incurring a multiplicative factor of $\mathcal{O}(\log(n))$ to their running time. These algorithms also require the embedding of a clique in $\mathbb{R}^K$, a task that demands $\mathcal{O}(K^3)$ time. If we assume K is not given as part of the input, then we can assume that K is $\mathcal{O}(n)$ (although tighter bounds exist [8]). Thus, any of these algorithms can be used within a bisection search for a total time of $\mathcal{O}(n^3 \log(n))$, in the worst case. We propose an algorithm which accomplishes the same task in $\mathcal{O}(n^3)$ time. If the embedding dimension is known, all algorithms (ours, as well as those in [1,6,7]) reduce to linear time in n.

Our algorithm is based on the problem of determining the intersection of K spheres in $\mathbb{R}^K$, where K varies during the algorithm. The problem of determining the intersections of spheres is well known, as are its applications (see, e.g. [2]). We numerically compare the algorithm with an existing technique

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