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An Introduction to Distance Geometry applied to Molecular Geometry

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Preface

Distance geometry (DG) is a distinct mathematical research area which includes mathematics and computer science as fundamental components. The fundamental problem of DG is to determine the spatial locations (coordinates) for a set of points, in a given geometric space, using distances between some of them.

DG is considered to have originated in 1928, when Menger [62] characterized several geometric concepts using the idea of distance [16]. However, only with the results of Blumenthal [10], in 1953, did the topic become a new area of knowledge known as DG.

The main challenge of DG at that time was to find necessary and sufficient conditions in order to decide if a given matrix is a distance matrix D. That is, decide whether or not a given matrix D is a symmetric matrix such that there is an integer number K and a set of points in $\mathbb{R}^K$, where the Euclidean distances between these points are equal to the entries of the matrix D [51]. Note that, in this case, all distances are considered known.

To the best of our knowledge, the first explicit mention of the fundamental problem of DG delineated above, where not all distances are known, was given by Yemini [81], in 1978. In this case, the problem may be harder.

Another important moment in the history of DG is related to its application to the calculation of molecular structures, with the 1988 publication of Crippen and Havel's book [15], considered pioneers of DG in the analysis of protein structures. More information on the DG history can be found in [52].

The first edited book fully dedicated to DG was published by Springer in 2013 [67]. The book brought together different applications and researchers in DG. In the same year, in June 2013, the first international workshop dedicated to DG was held with speakers from various international institutions (Princeton University, IBM TJ Watson Research Center, University of Cambridge, École Polytechnique, Institut Pasteur, École Normale Supérieure, SUTD-MIT International Design Center). The event also had the support of several international scientific societies and universities, indicating the importance of DG in many areas of knowledge (more details at http://dga2013.icomp.ufam.edu.br/).

The interest in DG as a topic of research arises from the wealth and diversity of its applications, in addition to its mathematical depth and beauty. Recent surveys on DG highlighting the theory and applications can be found in [9, 18, 57]. For example, applications can be found in problems from astronomy, biochemistry, statistics, nanotechnology, robotics, and telecommunications.

In astronomy, the problem is related to the determination of star positions using information about the distances between some of them [60]. In biochemistry, the problem appears in the determination of three-dimensional structures of protein molecules using the information obtained from nuclear magnetic resonance (NMR) experiments. In statistics, there are problems related to visualization of data [22] and dimensionality reduction [50]. In these cases, points and distances are given in a high dimensional space $\mathbb{R}^n$ and the problem is how represent them in a lower dimension, say $\mathbb{R}^2$ or $\mathbb{R}^3$, in order to have a visual idea of the data. This application is also linked to a current topic of research called *Big Data* [2, 61]. In nanotechnology, the problem is similar to the problem in biochemistry, but on a "nano" scale [21, 39]. There is a direct relationship between the application to robotics and the calculations related to molecular geometry [23, 70]. That is, given a set of robotic arm lengths (distances), the problem is to find the locus of points that the robot arm can reach [68]. In telecommunications, the problem is related to the positioning of a wireless sensor network, where the distances can be estimated by the amount of power necessary for performing peer-to-peer sensor communication. The further the sensors, the more power is necessary. Since both sensors know how much power they used, both sensors can compute their distance. An example of this is for router positioning [24, 81].

The theoretical nature and the wide variety of applications have resulted in DG becoming its own research area in applied mathematics, which includes fundamental concepts from mathematics (measures, norms, geometry, optimization, combinatorics, graph theory, symmetry, uncertainty) and computer science (algorithms, solvability, complexity).

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