Minissimpósio 11

Distance Geometry and Applications

Organizers:

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1 Description on the theme

Distance Geometry (DG) is the study of geometry with the main primitive concept being the notion of distance, instead of points and lines, for instance, which are the pillars of the classical approaches.

In 1928, Karl Menger (1902-1985) characterized various concepts such as congruence and convexity in terms of distances. These results were later complemented by Leonhard Blumenthal (1953) in a book that essentially inaugurated Distance Geometry as a subfield of Mathematics.

After a period without significant new records in literature, the biophysicist Gordon Crippen started using Distance Geometry results in protein conformation problems from 1977 onwards, achieving great success in

the development of mathematical-computational methods. This fact propelled this area as predominantly associated with Computational Mathematics and its applications.

In recent decades, this area has attracted researchers from other branches of Applied Mathematics and Computer Science whose interest lies in what is called the Distance Geometry Problem: *given a list of distances between pairs of objects, locate these objects in a geometric space in such a way that their pairwise distances coincide with those in the list.*

This problem finds several relevant applications such as Sensor Network Localization, Determination of Nanostructures and Protein Structures, Multidimensional Scaling, Graph Realization, Machine and Deep Learning, among others.

These applications have strengthened the interface of Distance Geometry with other areas of knowledge such as Bioinformatics, Robotics, Computing, and Data Science, as well as its interaction with subfields of mathematics like Geometric Algebra, Optimization, Graph Theory, and Operations Research.

2 Brief History and Goals

In this context, the aim of this mini-symposium proposal is to bring together researchers in Distance Geometry and related areas who can contribute to their development through the exchange of experiences and recent research results.

Among the guests, there will be an internationally renowned guest (Leo Liberti) who has clear prominence in the field's research and has been indicated to be a plenary speaker by some of the researchers of our community, along with national guests, including both well-established researchers and graduate students. This emphasizes the organizers' commitment to firmly establish this research area in the country, fostering the formation of new researchers and promoting the involvement of women in Applied and Computational Mathematics research, goals which aim to be achieved by our society (SBMAC).

This mini-symposium has already been held within CNMAC on four other occasions, specifically in 2018, 2019, 2021, and 2023. The encouragement for the annual occurrence of this mini-symposium aligns with the goal of consolidating the research area, as each year it adds new researchers with new theoretical ideas and applications, achieving great success.

3 Preliminar Program

It will consist of two sessions, each with four presentations, following the organization below.

Quinta-Feira (19 de setembro): 08h00 – 10h00 / *Moderação*: Felipe Fidalgo

1. **An Optimization-Based Approach to the Vector Geometry Problem with Computational Insights**

   Luiz Leduíno de Salles Neto
   Federal University of São Paulo (UNIFESP)

   Abstract: We have data on the differences between vectors in many practical situations, such as locating sensors or sources. The objective is to find the location of the vertices. This problem is called

the Vector Geometry Problem (VGP) and is somewhat related to the well-known Distance Geometry Problem (DGP). This work presents the definition, an optimization-based approach to solving the VGP, and the results obtained in the computational experiments.

2. **On the stationary points of S-STRESS function**

Douglas Soares Gonçalves
Department of Mathematics
Federal University of Santa Catarina (UFSC)

Abstract: We investigate some properties of stationary points of the Smooth STRESS (S-STRESS) function. Differently from the Raw-STRESS (or simply STRESS) well known in multidimensional scaling literature, it is still unclear whether S-STRESS admits local minimizers that are not global. By assuming that all distances are exact we show that under certain conditions all stationary points with function value greater than zero admit a direction of negative curvature and thus cannot be local minimizers. We hope these results may shed some light in this open problem in the field of distance geometry and multidimensional scaling.

3. **On some remarks on the resolution of Least Squares Problem in Conformal Geometric Algebra**

Emerson Vitor Castelani
Department of Mathematics
State University of Maringá (UEM)

Abstract: Consider the following problem: given a set of m points $\mathcal{Q} = \{Q_i \in \mathbb{R}^n; i \in \{1, ..., m\}\}$ and a set of objects $\mathcal{O} = \{$straight lines, hyperplanes, hyperspheres and hypercircles$\}$, the objective is to determine which object in $\mathcal{O}$ comes as close as possible, minimizing some algebraic distance between objects and points, from the set $\mathcal{Q}$.

The core of this problem lies in determining the minimum distances between a geometric object and a set of points in $\mathbb{R}^n$. Note that, in this problem, we added an additional condition in relation to the classical formulation of least squares problems. Although the classical least squares formulation of the object is predefined, requiring a determination of its parameters, no problem presented leaves open which object will be adjusted. One way to solve this type of problem is to model the object to be detected by a vector (or external product of vectors) of the conformal space.

There are two central approaches to solving this problem and both are based on determining an eigenvector associated with the smallest eigenvalue of a linear security operator. In practice, the use of Conformal Algebra is restricted to modeling, while the resolution takes place using Classical Linear Algebra. We will propose an alternative to existing approaches, maintaining the following characteristics: integrity of the modeling and resolution environment, consistency of the minimized distance and its geometric meaning, robustness and speed in obtaining the answer, and without the need to calculate eigenvalues.

4. **Intermolecular distance functions and their derivatives in internal coordinates - Part 2**

Jesus Marcos Camargo
West State University of Paraná (UNIOESTE)

Abstract: Intermolecular distance functions play a significant role in molecular dynamics problems. While the most direct method to obtain them involves using Cartesian coordinates, describing the molecule based on the spatial distribution of its atoms, variations in the positions of these atoms often result from changes in torsion angles, which are components of the set of internal coordinates. This reason motivated us to determine the analytical form of these functions and their derivatives in terms of internal coordinates. Furthermore, we have shown that by using homogeneous space, a representation of $\mathbb{R}^3$ within a space of dimension four, it is possible to achieve significant reductions and simplifications for such expressions. In this new presentation, we will explore how further expansion of the representation space (now to dimension five) can offer additional advantages in describing distance functions and their derivatives, restoring the orthogonality of the equations.

Sexta-Feira (20 de setembro): 08h00 – 10h00 / *Moderação*: Carlile Lavor

1. **A continuous optimization approach to the MDGP with interval distances**

Mariana da Rosa
University of Campinas (UNICAMP)

Abstract: In order to deal with interval distances in the Molecular Distance Geometry Problem (MDGP), we will discuss an iterative method based on the integration of a spectral gradient projection algorithm with a method of projection.

2. **A Branch-and-Prune algorithm with search based on protein pattern frequency**

Romulo Marques
University of Campinas (UNICAMP)

Abstract: Proteins are essential organic molecules in biological processes, and their functions are directly tied to their three-dimensional shapes. Mathematically, the problem of determining the 3D structure of protein molecules can be modeled as a Discretizable Distance Geometry Problem (DDGP). The term 'Discretizable' arises from the following fact: in a DDGP, the solution space can be organized into a binary tree, implying that this problem can be solved in an exact and discrete manner. The discrete method that solves a DDGP is called Branch-and-Prune (BP). BP explores the binary tree solution space through Depth-First Search (DFS): at each node of the tree, the method evaluates the child nodes of the current node before evaluating the sibling nodes, always assessing the left child node first. However, this approach to exploring the search tree makes little use of publicly available protein structure data.

In this study, we analyzed all instances derived from Nuclear Magnetic Resonance experiments present in the Protein Data Bank (PDB) (a sample of 14134 molecules). We found that the distribution of solutions for protein DDGPs is vastly different from a uniform distribution, indicating that Nature 'prefers' some patterns over others. We present a variation of the BP algorithm that, instead of exploring the DDGP solution space using Depth-First Search (DFS), navigates the binary tree giving preference to more probable solution patterns (Frequency-Based Search - FBS).

3. ***To be announced***

Michael Souza
Federal University of Ceará (UFC)

Abstract: *To be announced.*

4. **A special session on open problems on Distance Geometry and Applications**

Abstract: In this section, we propose the speakers to propose open problems in order to be discussed by the audience. This very same session happened last year in Bonito and it had a great success: new research links have been developed. Our intention is to repeat it in order to incentivate new collaborations among the researchers of the group and from the audience.