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GOR-Arbeitsgruppe: Praxis der Mathematischen Optimierung

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Herewith, we invite you to the 99th meeting of the GOR working group "Real World Mathematical Optimization" in the Physikzentrum Bad Honnef (Hauptstr. 5, 53604 Bad Honnef, http://www.pbh.de). This meeting is hold as a symposium with the topic

Distance Geometry: Inverse problems between geometry and optimization

The workshop takes place on November 23 & 24, 2017 a Thursday and Friday.

The working language will be English, since many speakers and participants come from abroad.

Note that the participation in a GOR-AG-Workshop for non-members is subject to a registration fee, unless you are a speaker or a host. Except for students, the Physics Center collects an infrastructure fee of 30 Euro/person.

Please register yourself online using https://www.redseat.de/pmo99/ as soon as possible, but ideally not later than October 28th, 2017. The latest information on the meeting is available on the homepage of the GOR (http://www.gor-ev.de/arbeitsgruppen/praxis-der-mathematischen-optimierung).

Yours sincerely,

Josef Kallrath, Jens Schulz, Julia Kallrath (GOR AG) & Leo Liberti (CNRS & Ecole Polytechnique) liberti@lix.polytechnique.fr

Distance Geometry – Inverse problems between geometry and optimization

This symposium is about real world optimization problems involving distance geometry (DG). Consider the very easy problem: given a set of points in a Euclidean space, compute a subset of the pairwise distances. The fundamental problem in DG is the corresponding inverse problem: given a simple undirected graph with edges weighted by the distance values, as well as an integer *K*, compute a set of points in a *K*-dimensional Euclidean space which realize the given distances. The corresponding decision problem (i.e. determine whether or not there exists the realization) is called Distance Geometry Problem (DGP).

Applications

This problem is crucial in several branches of science and engineering: synchronization protocols, positioning of wireless devices, structural biology, nanotechnology, control of unmanned underwater vehicles, graph drawing, architecture and more.

In synchronization protocols, a set of communicating devices have to exchange as little data as possible, while a central coordinating device must be able to work out the absolute time of each device in the network. This can be achieved by routing to the server the pairwise time difference for each connected device pair. The server can then reconstitute a weighted graph, and solve a DGP in one dimension in order to compute the absolute times.

A set of wireless devices moving in an office floor can work out pairwise distances by estimating the battery used in peer-to-peer communication (the nearest the pair, the closest). The information can be synthesized in a weighted graph. Any realization of this graph in the plane (two dimensions) provides a possible positioning of the wireless sensors.

The function of proteins is determined by both chemical configuration and geometric conformation of the atoms. Some of the inter-atomic distances can be estimated quite precisely by chemical considerations (e.g. bond lengths and bond angles will yield all weighted triangles in the graph). Other distances can be estimated using Nuclear Magnetic Resonance (NMR). This yields a weighted graph, the realization of which in three-dimensional space provides a possible conformation of the protein.

Studying nanostructures involves a variant of the DGP, called the *unassigned* DGP (uDGP). In this setting, retrieving the weighted graph from the NMR data is more difficult; the input to the uDGP is simply a sequence of distance values, without reference to their adjacencies. The uDGP asks to compute the realizations of the given sequence in 3D.

It is well known that GPS signals do not reach underwater. In a fleet of unmanned underwater vehicles focused on accomplishing a task, every submarine has to know the positions of the others at all times. They can estimate their respective distances by using their sonars; the correctness of the estimation depends on the distance itself. This yields a weighted distance graph that must be realized in 3D at each timestep.

Graph drawing refers to the representation of graphs in vector spaces of various kinds. The DGP is a graph drawing problem in Euclidean spaces of a given dimension *K*, where vertices are represented by points and edges by straight segments.

The application of architecture is somewhat different, as it does not concern the DGP proper; but, rather, the properties of the manifold of its solutions. One of the requirements of building architectural structures is that these must be able to stand even if subject to considerable external forces. Many architectural structures are modelled using *bars* of given length held together by devices called *joints* (some structures are actually built this way --- think of modern airport roofs). Weighted graphs are therefore appropriate abstract models for studying bar-and-joint architectural models. The main issue for any architectural structure is that it must not collapse. This notion, which is defined by forces acting on the bar-and-joint model, is called *rigidity* when applied to the weighted graph model. Although rigidity naturally applies to (graph,realization) pairs, a substantial theoretical body of research justifies the application of this notion to graphs, independently of the realization, at least in general. Graphs with finitely many realizations are rigid, while those with uncountably many realizations are flexible. Architectonically, the issue is that of having *redundant rigidity*: the guarantee that even if some of the bars break, the building will not collapse.

The impact of DG in applied mathematics

DG has been present in many sub-fields of mathematics.

- Heron's theorem, which establishes a formula for computing the area of a triangle given the side lengths, is a milestone of elementary geometry.
- L. Euler stated a famous conjecture that topologically described closed polyhedra are rigid. Cauchy gave an elegant proof of the case where the polyhedra are geometrically described as the intersection of a finite number of half-spaces, and specifically *strictly convex*. This proof was extended to the case of non-strictly convex polyhedra by Alexandrov. In 1978, Robert Connelly finally disproved the conjecture by exhibiting a flexible non-convex topologically described polyhedron.
- One of J.C. Maxwell's achievements was the graphical method for solving force diagrams. The method, based on a specific notion of duality for graphs drawn in the plane, achieves the balancing of degrees of freedom assigned to points and constraints imposed by segments in a way that is reminiscent to computations using the *rigidity matrix* of a graph.
- A. Cayley formalized an algebraic equation that describes the geometrical notion of a tetrahedron with zero volume. Although Cayley worked in given dimensions, his ideas are eminently generalizable. This generalization was accomplished by Carl Menger, who also developed the first unified theoretical body of work wholly on DG. Many algorithms today are based on the Cayley-Menger determinant. The work of Menger was eventually carried on by L. Blumenthal.
- The only non-logical and non-philosophical work of K. Gödel is in the field of DG. Among other things, Carl Menger was the founder of the renowned *Mathematische Kolloquium* in Vienna. Stimulated by DG talks given by Menger and some of his students, collaborators and seminar lecturers, responding directly to a question posed at a certain seminar, Gödel proved that if four points are realizable in 3D, then they are also realizable on th surface of a sphere with the given distances being the length of geodesic tetrahedron sides. The proof rests on a fixed-point theorem that looks more innocent than it turns out to be.
- One of the most important algorithms in *data science* is Multi-Dimensional Scaling (MDS). Informally, it can be described as follows: given some estimation of discrepancies between objects, it represents the object in Euclidean spaces so people can have a visual representation that helps them make informal decisions. Formally, MDS takes an approximate finite metric on n elements, turns it into an approximate *Gram matrix*, factors it, zeros the H negative eigenvalues, and takes the transpose of the factor to produce an $n \times H$ matrix representation of a realization in H dimensions. This algorithm rests on a theoretical discovery in DG made in 1935 by Isaac Schoenberg (who also invented *splines*), namely the formula linking each squared Euclidean Distance Matrix (EDM) D and the corresponding Gram matrix, i.e. $2B = J\,D\,J$, where $n\,J = n\,I - \mathbf{1}^{\mathsf{T}}\,\mathbf{1}$ and $\mathbf{1}$ is the all-one row vector.
- Another modern discovery used in data science and related to DG is the Johnson-Lindenstrauss Lemma (JLL). A wonderful piece of high-dimensional geometry which states something that is apparently very counter-intuitive, i.e.: for a finite set X of n points in an m-dimensional space and a given ε in (0,1) there exists a $K = O(\varepsilon^{-2} \ln n)$ and a $K \times m$ matrix T such that, for each pair of distinct x and y in X, we have $(1-\varepsilon)\ \|x - y\|_2 \leq \|T\,x - T\,y\|_2 \leq (1+\varepsilon)\|x - y\|_2$. Note that the embedding dimension K is independent of the original dimension m, which is surprising, and only depends on the natural logarithm of the number of points in X. This discovery has been used in clustering, unconstrained optimization, statistics and is currently being applied to constrained optimization.

Aim of the workshop

This two-day event attempts to give an overview of the current state-of-the-art of DG and of the development of its practical applications. Because of the many applications fields of DG, the theoretical knowledge is often mixed with the application's practical requirements. Many similar concepts have been defined more than once, and the communities around DG are segmented by the application. Among other things, we hope to contribute to unify these communities and help them to work together.

Please contact one of the organizers if you are interested in presenting at this workshop.

In talks, either 15+5 min, 25+5 min or 40+5 min by choice, experts from practice, research institutions or software companies, will present selected problems and the corresponding solutions. Experts from universities, research institutions, industry and software companies are welcome to present selected problems and available solutions. Since talk slots are limited, we reserve the right to select speakers.

Please contact:

Jens Schulz (jens.schulz@lhsystems.com), Julia Kallrath (julia.kallrath@h-da.de) or Josef Kallrath (josef.kallrath@web.de), or Leo Liberti (liberti@lix.polytechnique.fr) if you are interested in presenting.

Presentations from the following speakers have been confirmed:

Alexander Barvinok (University of Michigan, USA)
Convexity of the image of a quadratic map

Claudia D'Ambrosio (CNRS and Ecole Polytechnique, France)
Distance Geometry in linearizable norms, with applications

Ivan Dokmanic (Univ. of Illinois at Urbana-Champaign, USA)
Spatio-temporal distance matrices for kinetic point sets

Philip Duxbury (Michigan State University, USA)
Vector distance geometry: New reconstruction methods driven by experimental advances

Carlile Lavor (University of Campinas, Brazil)
Conformal Clifford Algebra and the Discretizable Molecular Distance Geometry Problem

Thérèse Malliavin (CNRS and Institut Pasteur, France)
Towards an application of the iBP algorithm to problems from structural biology

Antony Man-Cho-So (Chinese University of Hong Kong, China)
Generalized Power Method for Phase Synchronization with Provable Estimation and Convergence Guarantees

Antonio Mucherino (University of Rennes I, France)
Collaborative Dynamical Distance Geometry and Motion Adaptation

Maks Ovsjanikov (CNRS and Ecole Polytechnique, France)
Encoding and recovering the discrete metric on triangle meshes

Pierre-Louis Poirion (Huawei Research, France)
Optimal constraints aggregation method for ILP

Bernd Schulze (Lancaster University, UK)
Global rigidity of periodic structures

Ky Vu (Chinese University of Hong Kong, China)
TBA

Bradley Worley (Institut Pasteur, France)

Towards a probabilistic model of coupled rigid motions