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 will be in November 2017 on a Thursday and Friday.

The working language will be preferably English, since some speakers or participants are expected from abroad.

Please 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 40 Euro/person.

The latest information on the meeting is available on the homepage of the GOR (https://gor.uni-paderborn.de/index.php?id=54).

Yours sincerely,

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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.

Applications

This problem is crucial in several branches of science and engineering: synchronization protocols, positioning of wireless devices, structural biology, architecture and more (e.g. graph drawing, nanotechnology).

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.

Architecture

One of the requirements of building structures is that these must be able to stand even if subject to considerable external forces. If these structures are built using joints and bars of given length, a weighted graph is an appropriate model. Architecture is concerned with the *rigidity* (rather than the conformation) of such structures, i.e. the degrees of freedom of each node independently of the other nodes. The study of rigidity is intimately connected with the number of solutions of a given DGP instance: a graph is defined to be rigid if it has finitely many solutions modulo rotations and translations, and globally rigid if it has only one.

The impact of DG in applied mathematics

DG has a long history in mathematics, going back to Heron's theorem, through Euler's conjecture on the rigidity of polyhedra, Cauchy's proof of the conjecture in the convex case, Maxwell's force diagrams, and Cayley-Menger determinants, to the more modern results: a fixed-point theorem of Gödel about geodesic distances on a sphere, Schoenberg's link with positive semidefinite matrices, which is at the root of multidimensional scaling, as well as the latest advances in global optimization, semidefinite programming, and the mixed-combinatorial methods used in reconstructing protein conformation.

Aim of the workshop

This two-day event attempts to give an overview of the current state-of-the-art of distance geometry and its applications in practice. 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. We thus 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, each approx. 40 to 50 minutes, experts from practice, research institutions or software companies, will present selected problems and the corresponding solutions.