DIMACS Workshop on

Distance Geometry

Theory and Applications

Proceedings edited by Leo Liberti
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26-29 July 2016 at DIMACS, Rutgers University, NJ

Scientific Committee

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Farid Alizadeh, *Rutgers University, USA*
Tami Carpenter, *DIMACS, Rutgers University, USA*
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Rebecca Wright, *DIMACS, Rutgers University, USA*

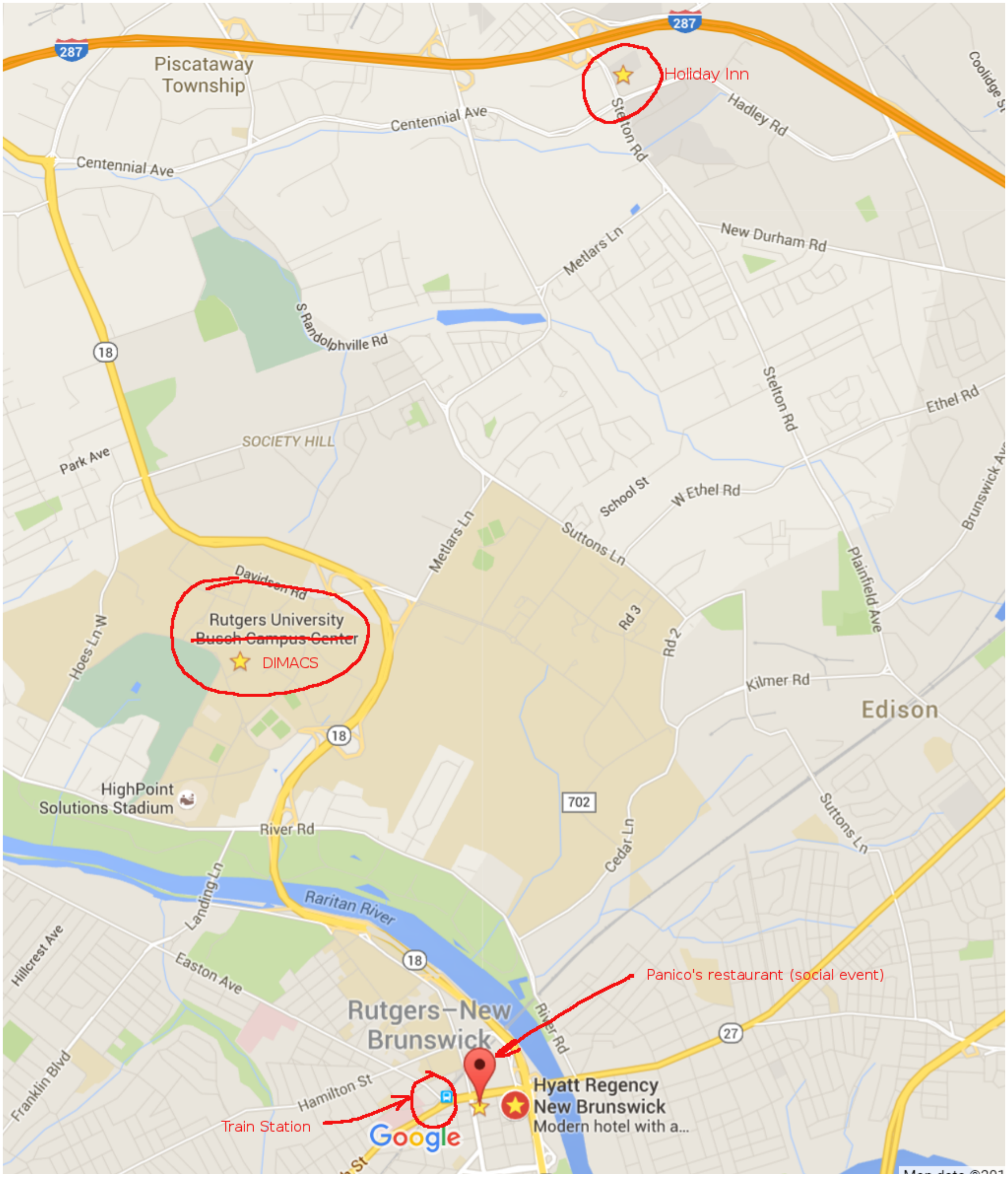
Materials from the workshop are available on the workshop website (`dimacs.rutgers.edu/Workshops/Distance`). We are videotaping the four tutorial presentations, and the videos will be posted on the website when they are available.

We gratefully acknowledge support from the National Science Foundation through awards DMS-1623007 and CCF-1144502.

Timetable

Tue 26 July		Wed 27 July "Tutorial day"		Thu 28 July		Fri 29 July	
0800-0850 0850-0900	*breakfast and registration* *Welcome*	0815-0840	*brkfast/registr*	0830-0900	*brkfast/registr*	0830-0900	*brkfast/registr*
0900-0930 0930-1000	Fampa Varvitsiotis	0840-1000	Jackson	0900-0930 0930-1000	Fawzi Parmenter	0900-0930 0930-1000	Hall Khoo
1000-1030	*pause*	1000-1030	*pause*	1000-1030	*pause*	1000-1030	*pause*
1030-1110 1110-1150	Lee Connelly	1030-1150	Streinu	1030-1110 1110-1150	Gortler Billinge	1030-1110 1110-1150	Sitharam Alfakih
1150-1350	*lunch*	1150-1400	*lunch*	1150-1420	*lunch*	1150-1420	*lunch*
1350-1400 1400-1430 1430-1500 1500-1530	*DIMACS Welcome by T. Carpenter* Gonçalves Krislock Malliavin	1400-1520	Wolkowicz	1350-1420 1420-1500 1500-1530	Lavor Jordan Singer	1420-1500 1500-1530	Man-Cho So Tanigawa
1530-1550	*pause*	1520-1540	*pause*	1530-1550	*pause*	1530-1535	*Closing*
1550-1620 1620-1700	Kalantari Szwarcfiter	1540-1700	Parrilo	1550-1620 1620-1700	Ozyesil Vetterli		
after 5pm	*reception at Panico's 103 Church St.*						

Finding your way around campus



This map points out the five spots that are of interest for DGTA16 (see next page).

The following sites are shown on the map in the previous page.

- DIMACS is in the CoRE building on the Busch Campus of Rutgers University. Parking permits will be available at the registration table on the day of the workshop. Please park in lot 64 located between the CoRE Building and the Werblin Recreation Center. If you are using a GPS to locate the parking lot, we suggest that you enter 98 Brett Road, Piscataway, NJ as the address. (The address for the CoRE building will take you to the building's main entrance, which does not have parking.) Be mindful: Google Maps does not seem to be able to locate "DIMACS"; instead, I search for "core building frelinghuysen road".
- The *New Brunswick* train station: it serves Amtrak and NJ Transit trains on the Northeast Corridor (`www.njtransit.com/pdf/rail/R0070.pdf`). Catch these trains from Penn Station in NYC or from Newark Airport station. Likely final destinations (from both Penn and Newark) are Princeton Junction, Hamilton, Trenton. Make sure your train stops at New Brunswick, and buy a ticket before boarding the train.
- The Panico's Italian restaurant (favourite choice within DIMACS, apparently — as an Italian, I take no responsibility!) where they organized the social event on tuesday night.
- The Hyatt Regency and Holiday Inn hotels (both used by attendees): 2.4 miles and 3.8 miles from DIMACS, respectively, so don't try walking these distances in the july heat (or storm, whichever happens to be the case). Ask your hotel for shuttle services; call taxis or ubers, or perhaps rent a bike. See `dimacs.rutgers.edu/Workshops/general/accommodations.html` for more information about shuttles.

The Rutgers University campus is quite large. I personally advise using Google Maps or, if you don't have a data plan in the USA but have a smartphone, download the `maps.me` app and the New Jersey offline map.

Distance Geometry Theory and Application

A DIMACS Workshop

Leo Liberti, *CNRS LIX, Ecole Polytechnique, 91128 Palaiseau, France*
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Welcome to this workshop, dedicated to Distance Geometry (DG), hosted (and organized) by DIMACS. I am most thankful to the extremely efficient DIMACS staff, particularly to Tami Carpenter, its Associate Director, for her incredible dedication. I am also extremely thankful to my co-chair, Farid Alizadeh, for securing some much-needed NSF funding. This workshop is the first about DG organized in the USA, but two other workshops about DG have been organized by Carlile Lavor in Brazil: in 2013 near Manaus and in 2014 in Campinas. There is no formal "steering committee", but I am always on the look-out for potential organizers of future DG workshops. So, if you are interested, please let me know.

A special issue dedicated to this workshop and to DG in general will be published in Discrete Applied Mathematics (DAM). While there is no firm submission deadline yet, the end of 2016 seems like a good date. I hope most of you will submit papers to this issue.

In Euclid's original view, geometry was based on points and lines. This view was brought forward by Descartes, who gave a more quantitative interpretation of points with the Cartesian plane and its axes. Calculus, mathematical analysis, linear algebra all make use of a concept of geometry which is based on points (sometimes called vectors). And yet, when Greek farmers squabbled over the extent of their triangular fields, they had an easier time calculating the side lengths rather than the coordinates of the vertices. The Alexandria colons circa 50AD seemed to be the most belligerent, and brought their fights before the wise Heron, who, tired of the hellish waste of time, devised a formula for computing the area of a triangle using nothing but the side lengths (forget the "base" and the "height", which always confused all of the farmers). We might as well ascribe to Heron the official birth of DG, although some would insinuate that similar methods for estimating the area of triangles were present in Egypt well before 50AD.

A few centuries later, Arthur Cayley took Heron's formula for triangles in the plane and generalized it, through a determinant, to simplex volumes in any dimension. Karl Menger, who worked at the beginning of the 20th century, and was fascinated by the (then) fashionable axiomatization of mathematics, picked up on the Cayley determinant and used it to try his own axiomatization of geometry through distances: so that, now, the Cayley determinant is actually called "Caley-Menger determinant[1]"

Menger, who is best known for organizing a popular seminar in Vienna in contrast to the Vienna Circle, who had become politicized and downright dangerous, apparently only made a single disciple[2] with his work on DG: Leonard Blumenthal. Blumenthal devoted his life to clarify the work of his advisor, which remained obscure both in the German original and in (his

[1] This was probably Menger's smartest career move.

[2] Who was also his Ph.D. student — he probably didn't have much of a choice.

own) English translation. So obscure, in fact, that attempts at explaining it are still ongoing.[3] Mathematical historians today are puzzled as to why Menger chose an axiomatization of geometry by distances. An accredited theory ascribes the reason to all of the other axiomatizations having been already taken by people like Hilbert, Bernays, Tarski (whose productivity between love affairs must be in the Guinness book of records), or Carnap (who axiomatized absolutely everything, including his interactions with his baker, who kept selling him multi-grain when he clearly wanted baguettes).

While giving M.Sc. level courses at the University of Vienna, Menger welcomed to his class a student who then became one of the most celebrated mathematicians of all time, Kurt Gödel. Gödel proved two incredibly deep theorems as a Ph.D. student: his *completeness theorem*, which states that any logically valid first-order formula has a formal proof, and his *incompleteness theorem*, which perversely states that there are true first-order formulæ which cannot have a proof.[4] Even more incredibly, Gödel never had a Ph.D. student, nor a co-author, except for a single paper[5] on DG, where he gives a devious fixed point argument to show that if four points can be realized in $\mathbb{R}^3$ (but not in $\mathbb{R}^2$), then they can also be realized on the surface of a sphere with geodesic curved sides having the same lengths.

This highly accurate (ehm) historical account did nothing so far to justify a contemporary interest in DG. So why should we have a workshop on it? Two breakthroughs, both related to the "Big Data" buzzword, will give us a better motivation. Isaac Schoenberg, the inventor of splines, unearthed in 1935 the relationship between Euclidean Distance Matrices (EDM) and positive semidefinite (PSD) matrices. This gave rise to the incredibly successful *multidimensional scaling* (MDS) technique for visualizing high-dimensional data. Schoenberg's paper bears the title *Remarks to Maurice Frechet's Article "Sur La Definition Axiomatique D'Une Classe D'Espace Distances Vectoriellement Applicable Sur L'Espace De Hilbert"*. What is really remarkable about Schoeberg's remarks is that no-one even remembers Fréchet's original paper, but everyone uses MDS.

The second breakthrough follows a similar pattern: Johnson and Lindenstrauss' 1984 paper *Extensions of Lipschitz mappings into a Hilbert space* focuses on a rather complex theorem concerning infinite dimensional spaces. To prove the theorem, the authors spend a couple of pages on a surprising lemma, now called the *Johnson-Lindenstrauss Lemma* (JLL). The JLL states that, given a set X of n vectors in $\mathbb{R}^m$, you can pre-multiply the vectors by a $k \times m$ matrix T where each component is sampled from a normal distribution with zero mean and $\frac{1}{k}$ variance, and, provided k is $O(\epsilon^{-2} \ln n)$ with some given $\epsilon \in (0,1)$, you get:

$$\forall x, y \in X \quad (1-\epsilon)\|x-y\|_2 \le \|Tx - Ty\|_2 \le (1+\epsilon)\|x-y\|_2.$$

Why is this surprising? Well, suppose you want to cluster 100,000 images using the k-means algorithm, which uses nothing but Euclidean distances. The thumbnail 100×100 RGB images

[3]See [Liberti & Lavor, *Six mathematical gems from the history of distance geometry*, to appear in ITOR] and [Bowers & Bowers, *A Menger Redux: Embedding metric spaces isometrically*, hopefully accepted in the American Mathematical Monthly].

[4]Explaining away the apparent contradiction in terms between the completeness and incompleteness theorems is left as an "easy exercise" for the reader — allowed solution time: approximately 2 years.

[5]Calling this work a "paper" is overkill — it is more like a one page abstract in Menger's seminar proceedings.

are actually vectors in $\mathbb{R}^{30,000}$. Now, if you set an error tolerance at 10%, i.e. $\epsilon = 0.1$, you could pick k to be around $100 \times \ln(100,000) \approx 1152$. So, instead of working with vectors having thirty thousand components, you could work with vectors having just over a thousand components. And, since k-means is only a heuristic, who knows whether the 10% error is even hurting your results? In other words, this is an eminently sellable technique, and I think that Google, Yahoo!, and Facebook are likely to use it a lot.[6] As I said, the JLL follows the same pattern as Schoenberg's paper: no-one remembers the actual theorem, but everyone knows the lemma.

But DG is not just "pure DG". In fact architecture, statics, and the worry of engineers that their next bridge might collapse and they might be sent to prison or worse, pushed the discipline towards another direction: what structures are resilient to external forces? I.e. what bar-and-joint structures are rigid or flexible? Rigid structures will only have finitely many incongruent realizations in space, whereas flexible structures will flex, and hence have uncountably many. Maxwell defined "force diagrams" based on rigidity notions, and a graphical algorithm to solve them. A famous 1766 conjecture of Euler's stated that all three-dimensional polyhedra must be rigid. As shown in a wonderful[7] proof by Cauchy, Euler was right insofar as one uses the definition of polyhedron as an intersection of half-spaces. But if one is willing to consider face incidence lattice based definitions, then a "polyhedron" might also be a nonconvex set. One of the speakers in this conference, Bob Connelly, the proud inventor[8] of a flexible (triangulated) sphere, has the peculiar distinction of having proved Euler wrong.

Motivationwise, that is not all. With the advent of computers, much of the number-crunching that no-one could have ever carried out by hand became possible. Today we can use DG-based methods for synchronizing clocks (thanks to Amit Singer), for localizing mobile sensors in wireless networks (thanks to a bunch of people, including Henry Wolkowicz and Nathan Krislock), for finding the shape of proteins using Nuclear Magnetic Resonance (NMR) distance data (thanks to an even larger bunch of people, including Carlile Lavor, Douglas Gonçalves, Thérèse Malliavin, Simon Billinge, Yuehaw Khoo), and for other applications.[9]

For more information about DG, I will shamelessly refer you to my own survey[10], and also, more honorably, to the wonderful survey[11] written by Martin Vetterli and his co-authors.

[6] This belief is based on the sound assumption that if I were them, I would use this technique a lot.

[7] If only very slightly wrong...

[8] I am going to use the latin meaning of "inventor", i.e. "he who finds", rather than the most common meaning of "constructor of a new idea".

[9] Not all DG applications are well represented at this workshop, but not for my lack of trying! But as these DG workshops keep happening, I am sure we will reach *all* DG applications out there.

[10] See [Liberti et al., *Euclidean Distance Geometry and Applications*, SIAM Review 56(1):3-69, 2014].

[11] See [Dokmanic et al., *Euclidean Distance Matrices: Essential theory, algorithms and applications*, IEEE Signal Processing Magazine, 1053-5888, 12-30, 2015].

Abstracts

1. Tue 26 July, 9-9:30

Marcia Fampa, *COPPE, Federal University of Rio de Janeiro, Brazil*

Modeling the Euclidean Steiner Tree problem

In the Euclidean Steiner Tree Problem, the goal is to find a network of minimum length interconnecting a set P of given points in the n-dimensional Euclidean space. Such networks may be represented by a tree T, where the set of nodes is given by the points in P, known as terminals, and possibly by additional points, known as Steiner points. The length of the network is defined as the sum of the Euclidean lengths of the edges in T. We will present mixed integer nonlinear programming formulations for the problem from the literature, and discuss the difficulties involved in solving them by branch-and-bound algorithms. Different techniques to overcome these difficulties are proposed and some numerical results show their impact on the solution of the problem.

(Joint work with Claudia D'Ambrosio, Jon Lee, Nelson Maculan, Wendel Melo and Stefan Vigerske.)

2. Tue 26 July, 9:30-10

Antonios Varvitsiotis, *NTU Singapore*

Graph Cores via Universal Completability

A framework for a graph $G = (V, E)$, denoted $G(p)$, consists of an assignment of real vectors $p = (p_1, p_2, ..., p_n)$, where $n = |V|$, to its vertices. A framework $G(p)$ is called universally completable if for any other framework $G(q)$ that satisfies $p_i^\top p_j = q_i^\top q_j$ for all $i = j$ and (i, j) in E there exists an isometry U such that $Uq_i = p_i$ for all i in V. A graph is called a core if all its endomorphisms are automorphisms. In this work we identify a new sufficient condition for showing that a graph is a core in terms of the universal completability of an appropriate framework for the graph. To use this condition we develop a method for constructing universally completable frameworks based on the eigenvectors for the smallest eigenspace of the graph. This allows us to recover the known result that the Kneser graph $K_{n:r}$ and the q-Kneser graph $qK_{n:r}$ are cores for $n \geq 2r + 1$. Our proof is simple and does not rely on the use of an Erdös-Ko-Rado type result as do existing proofs. Furthermore, we also show that a new family of graphs from the binary Hamming scheme are cores, which was not known before.

(Joint work with Chris Godsil, David Roberson, Brendan Rooney and Robert Šámal.)

3. Tue 26 July, 10:30-11:10

   Jon Lee, *University of Michigan, USA*

   ### Relaxing kindly and efficiently

   Very generously interpreting the conference theme, I will talk about two issues that arise in the sBB (spatial branch-and-bound) global-optimization algorithm. One has to do with smoothing functions having limited non-differentiability (for example, p-th roots which arise in computing distances via p-norms) in a suitable way for sBB. The second has to do with a way of measuring quality of convex relaxations via volumes and getting from the mathematical analysis, some actionable algorithmic ideas for sBB.

4. Tue 26 July, 11:10-11:50

   Bob Connelly, *Cornell University, USA*

   ### Global rigidity and universal rigidity of bipartite graphs

   A framework, given by a graph together with a configuration of its vertices, is globally rigid in Euclidean space if every other configuration, with the corresponding edge lengths the same, is congruent to the original. We will show that for complete bipartite graphs in d-space, if the configuration is generic and the partitions cannot be separated by quadric surfaces, then not only is the framework globally rigid in d-space, but it is globally rigid in all higher dimensions as well, a property called universal rigidity. Using geometric criteria it is possible to give many concrete examples of bipartite frameworks that are universally rigid.

   (Joint work with Steven Gortler and Louis Theran.)

5. Tue 26 July, 2pm-2:30pm

   Douglas Gonçalves, *Federal University of Santa Catalina, Brazil*

   ### A least-squares approach for the discretizable distance geometry problem with inexact distances

   The discretizable distance geometry problem in dimension K is a particular case of the distance geometry problem in which there exists a vertex order ensuring that the initial K vertices form a clique and for the remaining vertices, there are at least K reference distances to predecessors. We extend a branch-and-prune approach for this problem by considering noisy distances instead of exact ones. Candidate positions are obtained by the solution of a least-squares problem related to a reduced distance matrix, and possibly by a reflection around the affine subspace generated by the references. The feasibility of such candidates is verified based on a perturbation result for the singular value decomposition and the discrepancy principle.

6. Tue 26 July, 2:30pm-3pm

   Nathan Krislock, *Northern Illinois University, USA*

   ### Facial reduction for Euclidean distance matrix problems

   A powerful approach to solving problems involving Euclidean distance matrices (EDMs) is to represent the EDM using a semidefinite matrix. Due to the nature of these problems, the resulting semidefinite programming problem is typically not strictly feasible. In this talk we discuss how to take advantage of this lack of strict feasibility by using facial reduction to obtain smaller equivalent problems. This approach has proven very successful for solving large-scale Euclidean distance matrix problems having little to no noise in the given incomplete distance measurements. We will present recent results on the use of facial reduction for solving noisy Euclidean distance matrix problems.

7. Tue 26 July, 3pm-3:30pm

   Thérèse Malliavin, *CNRS & Institut Pasteur, France*

   ### The interval Branch-and-Prune algorithm for the Molecular Distance Geometry Problem: towards an application to real-life protein structure determination by NMR

   The interval branch-and-prune (iBP) approach has been proposed ([1-6]) as a method for allowing a global optimisation of molecular structure with distance restraints. A recursive implementation of this algorithm [9] has allowed the application of this approach to small structures of proteins in alpha-bundles. Here, we are going to present the results obtained on a set of protein structures with sizes from 24 to 120 residues, displaying various secondary structures and topologies. The results obtained with various sets of distance restraints, including exact values and intervals of values, will be presented, in order to experimentally evaluate the complexity of the algorithm on real-life cases of protein structure determination. This experimental evaluation will be related to the theoretical estimation previously obtained in [8]. The effect of several acceleration procedures will be used in order to allow a complete exploration of the tree describing the solutions of Molecular Distance Geometry Problem instances. The consequences of the availability of such an approach for the field of structural biology will be discussed [7].

   [1] Lavor C., Liberti L., Mucherino A., *On the solution of molecular distance geometry problems with interval data*, in Proceedings of the InternationalWorkshop on Computational Proteomics (Int. Conf. on Bioinformatics and Biomedicine), IEEE, Hong-Kong, 77-82, 2010.

   [2] Liberti L., Lavor C., Maculan N., *A branch-and-prune algorithm for the molecular distance geometry problem*, International Transactions in Operational Research, 15:1–17, 2008.

   [3] Lavor C., Liberti L., Maculan N., Mucherino A., *The discretizable molecular distance geometry problem*, Computational Optimization and Applications (2012) 52:115–

146.

[4] Lavor C., Liberti L., Mucherino A., *The interval Branch-and-Prune algorithm for the Discretizable Molecular Distance Geometry Problem with inexact distances,* Journal of Global Optimization, 56:855-871, 2013.

[5] Lavor C., Alves R., Figueiredo W., Petraglia A., Maculan N., *Clifford Algebra and the Discretizable Molecular Distance Geometry Problem,* Advances in Applied Clifford Algebras 25 (2015), 925–942.

[6] Mucherino A., Lavor C., Malliavin T., Liberti L., Nilges M., Maculan N., *Influence of Pruning Devices on the Solution of Molecular Distance Geometry Problems,* in Pardalos, P. and Rebennack, S. (eds.), Experimental Algorithms (ISCO), LNCS 6630:206-217, 2011.

[7] Malliavin T.E., Mucherino A., Nilges M., *Distance geometry in structural biology: new perspectives,* in A. Mucherino et al. (eds.), Distance Geometry: Theory, Methods and Applications, Springer, 2013.

[8] Liberti L., Lavor C., Mucherino A., *The Discretizable Molecular Distance Geometry Problem Seems Easier on Proteins,* in A. Mucherino et al. (eds.), Distance Geometry: Theory, Methods and Applications, Springer, 2013.

[9] Cassioli A., Bardiaux B., Bouvier G., Mucherino A., Alves R., Liberti L., Nilges M., Lavor C. and Malliavin T., *An algorithm to enumerate all possible protein conformations verifying a set of distance constraints,* BMC Bioinformatics 28:16-23, 2015.

(Joint work with M. Machat, B. Bardiaux, A. Cassioli, C. Lavor, L. Liberti.)

8. Tue 26 July, 3:50pm-4:20pm

Bahman Kalantari, *Comp. Sci. Dept., Rutgers University, USA*

The Triangle Algorithm: An Algorithmic Separation Theorem and its Application

First, we introduce the Triangle Algorithm, a fully polynomial time approximation scheme (FPTAS) for the convex hull membership problem (CHMP). CHMP is testing if the convex hull of a finite set of points in the Euclidean space contains a distinguished point, a fundamental problem in LP, statistics, machine learning and computational geometry. The validity of the algorithm relies on a geometric duality, called distance duality. Next, we describe a generalization of the Triangle Algorithm, the distance duality and corresponding computational complexities for testing if two arbitrary compact convex subsets K and K' intersect. It computes p in K and p' in K', where either the Euclidean distance $d(p, p')$ is arbitrarily small, or the orthogonal bisecting hyperplane to the line segment pp' separates K from K'. If desired, it computes the optimal supporting hyperplanes. It thus applies to the support vector machine (SVM) problem. Having tested the Triangle Algorithm on reasonably large size instances of CHMP, LP, and SVM, it is competitive with the Frank-Wolfe method, the simplex method, and the sequential minimal optimization algorithm (SMO). In fact in an unorthodox application of the Triangle Algorithm in solving a linear system, it outperforms such iterative methods as SOR and AOR.

It also finds applications in solving relaxations of NP-hard problems. In summary, the Triangle Algorithm is a robust algorithm that finds applications in diverse problems in optimization, CS and numerical analysis.

9. Tue 26 July, 4:20pm-5:00pm
Jayme Szwarcfiter, *Federal University of Rio de Janeiro, Brazil*

On graph convexities related to paths and distances

A graph convexity is a pair $(G, \mathcal{C})$, where G is a finite graph with vertex $V(G)$ and $\mathcal{C}$ a family of subsets of $V(G)$ satisfying $\varnothing, V(G) \in \mathcal{C}$ and being closed under intersections. The sets $C \in \mathcal{C}$ are called *convex sets*. The most common graph convexities are those whose convex sets are defined through special paths of the graph. Among them the most prominent are the *geodesic convexity*, where $\mathcal{C}$ is closed under taking shortest paths, the *monophonic convexity*, where $\mathcal{C}$ is closed under induced paths and the P_3 convexity, whose convex sets are closed under pairs of common neighbors. We examine some common parameters of graph convexities, as the *geodetic number, convexity number, hull number, Helly number, Carathéodory number, Radon number and rank*. In particular, we describe complexity results related to the computation of these parameters.

10. Wed 27 July, 8:40-10:00

Bill Jackson, *Queen Mary University of London, UK*

Rigidity and Global Rigidity of Frameworks (*tutorial*)

The study of the rigidity of frameworks has its origins in the work of Euler, Cauchy and Maxwell. There was a flurry of activity in the 1970's prompted by Laman's characterisation of rigid generic bar-joint frameworks in the plane and Connelly's counterexample to Euler's original conjecture on rigid polyhedra in 3-space. This activity has increased since then and it is now an exciting and thriving research area. I will give an introduction to rigidity theory, concentrating on results and problems for bar-joint frameworks but also describing how these have been extended to other types of frameworks and the matrix completion problem.

11. Wed 27 July, 10:30-11:50

Ileana Streinu, *Smith College, USA*

Periodic Rigidity: a Survey (*tutorial*)

A periodic bar-and-joint framework is an abstraction of atom-and-bond crystal structures. Following a general introduction to the deformation theory of this type of frameworks (introduced in 2010 by Ciprian Borcea and the speaker), I will survey results on Maxwell-type characterizations, the connection to rigidity theory for finite frameworks as well as applications to expansive and auxetic periodic structures.

12. Wed 27 July, 2pm-3:20pm

Henry Wolkowicz, *University of Waterloo, Canada*

Facial Reduction in Cone Optimization with Applications to Matrix Completions

Slater's condition – existence of a "strictly feasible solution" – is at the heart of convex optimization. It is enough to look at the basics: without strict feasibility, first-order optimality conditions may be meaningless, the dual problem may yield little information about the primal, and small changes in the data may render the problem infeasible. In consequence, many off-the-shelf numerical methods can perform poorly; primal-dual interior point methods, in particular. New optimization modelling techniques and convex relaxations for hard nonconvex problems have shown that the loss of strict feasibility is a much more pronounced phenomenon than has previously been realized. Such new developments suggest a reappraisal. In this talk we describe the various reasons for the loss of strict feasibility, whether due to poor modelling choices or (more interestingly) rich underlying structure, and describe ways to cope with it.

In particular, we look at three different views: (i) from the ground set of the application; (ii) from the lifted space of semidefinite matrices in the relaxation; (iii) from the image space of the relaxation.

We consider applications to Euclidean matrix completions for sensor network localization and molecular conformation problems.

(Joint work with Dmitriy Drusvyatskiy.)

13. Wed 27 July, 3:40pm-5pm

Pablo Parrilo, *MIT, USA*

Graph structure in polynomial systems: Chordal networks

The sparsity structure of a system of polynomial equations or an optimization problem can be naturally described by a graph summarizing the interactions among the decision variables. It is natural to wonder whether the structure of this graph might help in computational algebraic geometry tasks (e.g., in solving the system). In this lecture we will provide a gentle introduction to this area, focused on the key notions of chordality and treewidth, which are of great importance in related areas such as numerical linear algebra, database theory, constraint satisfaction, and graphical models. In particular, we will discuss "chordal networks", a novel representation of structured polynomial systems that provides a computationally convenient decomposition of a polynomial ideal into simpler (triangular) polynomial sets, while maintaining its underlying graphical structure. As we will illustrate through examples from different application domains, algorithms based on chordal networks can significantly outperform existing techniques.

(Joint work with Diego Cifuentes.)

14. Thu 28 July, 9-9:30

Hamza Fawzi, *MIT, USA*

Positive Semidefinite Rank

Let M be a $p \times q$ matrix with nonnegative entries. The positive semidefinite rank (psd rank) of M is the smallest integer k for which there exist positive semidefinite matrices A_i, B_j of size $k \times k$ such that $M_{ij} = \mathsf{trace}(A_i\, B_j)$. The psd rank plays an important role in semidefinite optimization in the context of semidefinite representation of polytopes. In this talk I will describe this connection and will outline some of the main properties and open questions concerning the psd rank.

(Joint work with João Gouveia, Pablo Parrilo, Richard Robinson, James Saunderson, Rekha Thomas.)

15. Thu 28 July, 9:30-10

Frank Permenter, *MIT, USA*

Dimension Reduction For SDPs Via Jordan Algebras

We propose a new method for simplifying semidefinite programs inspired by symmetry reduction. Specifically, we show if a projection satisfies certain invariance conditions, restricting to its range yields an equivalent primal-dual pair over a lower-dimensional symmetric cone—namely, the cone-of-squares of a Jordan subalgebra of symmetric matrices. We then give a simple algorithm for minimizing the rank of this projection and hence the dimension of this cone. Finally, we explore connections with *-algebra-based reduction methods, which, along with symmetry reduction, can be seen as special cases of our method.

16. Thu 28 July, 10:30-11:10

Steven Gortler, *Harvard University, USA*

Affine rigidity and Conics at Infinity

We prove that if a framework of a graph is neighborhood affine rigid in d-dimensions (or has the stronger property of having an equilibrium stress matrix of rank $n-d-1$) then its edge directions lie on a conic at infinity if and only if the framework is ruled on a single quadric. This strengthens and also simplifies a related result by Alfakih. It also allows us to prove that the property of super stability is invariant with respect to projective transforms and also to the coning and slicing operations. Finally this allows us to unify some previous results on the Strong Arnold Property of matrices.

(Joint work with Bob Connelly and Louis Theran.)

17. Thu 28 July, 11:10-11:50

Simon Billinge, *Columbia University, USA*

The Unassigned Distance Geometry Problem Applied to Find Atoms in Nanoclusters for Sustainable Energy

Studies of distance geometry problems (DGP) have focused on cases where the vertices at the ends of all or most of the given distances are known or assigned, which we call assigned distance geometry problems (aDGPs). The problem can get much more difficult when the vertices at the end of each edge are not known, the case we call the unassigned distance geometry problem (uDGP).

There is a pressing practical problem that is a realization of this case: finding the atomic structure of molecules and nanoparticles using X-ray or neutron diffraction data from non-crystalline materials. In this talk I will review the nanostructure inverse problem and its graph theoretical description, and describe some progress that has been made using build-up algorithms for discovering unassigned graph structures constrained by experimental results. I will also discuss limitations of the approach for real data with noise and measured with finite resolution, that makes these buildup problems inherently ill-posed.

(Joint work with Philip Duxbury and Pavol Juhas.)

18. Thu 28 July, 1:50pm-2:20pm

Carlile Lavor, *IMECC, University of Campinas, Brazil*

Distance Geometry and Clifford Algebra

Distance Geometry (DG) is the study of geometry based on the concept of distance and Clifford Algebra (CA) is a generalization of the hypercomplex number systems based on the concept of multivector. This talk will explain how DG and CA can be combined to model problems related to 3D protein structure determination using Nuclear Magnetic Resonance data.

19. Thu 28 July, 2:20pm-3

Tibor Jordan, *Eötvös Lorand University, Hungary*

Generic Global Rigidity of Graphs

A d-dimensional bar-and-joint framework is said to be globally rigid if every d-dimensional framework with the same underlying graph and with the same edge lengths is congruent to it. It is known that, for every fixed d, if the set of the joint coordinates is generic then global rigidity depends only on the underlying graph.

A major combinatorial question, which is still open in three-space and in higher dimensions, is whether there is a good characterization of the generically globally rigid graphs.

In this talk we shall give a survey of the known results and open questions concerning (a number of versions of) this question.

20. Thu 28 July, 3pm-3:30

Amit Singer, *Princeton University, USA*

Non-unique Games Over Compact Groups and Orientation Estimation in Cryo-EM

Let G be a compact group and let f_{ij} be real valued bandlimited functions over G for $i, j \in \{1, \ldots, n\}$. We define the Non-Unique Games (NUG) problem as finding $g_1, \ldots, g_n$ in G that minimize $\sum_{i,j=1}^{n} f_{ij}(g_i g_j^{-1})$. We devise a relaxation of the NUG problem to a semidefinite program (SDP) by taking the Fourier transform of f_{ij} over G. The NUG framework can be seen as a generalization of the little Grothendieck problem over the orthogonal group and the Unique Games problem and includes many practically relevant problems, such as orientation estimation in cryo-electron microscopy.

(Joint work with Yutong Chen and Afonso Bandeira.)

21. Thu 28 July, 3:50-4:20

Onur Ozyesil, *Princeton University*

Robust Camera Location Estimation by Convex Programming

3D structure recovery from a collection of 2D images requires the estimation of the camera locations and orientations, i.e. the camera motion. For large, irregular collections of images, existing methods for the location estimation part, which can be formulated as the inverse problem of estimating n locations $\mathrm{t}_1, \mathrm{t}_2, \ldots, \mathrm{t}_n$ in $\mathbb{R}^3$ from noisy measurements of a subset of the pairwise directions $\frac{\mathrm{t}_i - \mathrm{t}_j}{\|\mathrm{t}_i - \mathrm{t}_j\|}$, are sensitive to outliers in direction measurements. In our work, we firstly provide a complete characterization of well-posed instances of the location estimation problem, by presenting its relation to the existing theory of parallel rigidity. For robust estimation of camera locations, we introduce a two-step approach, comprised of a pairwise direction estimation method robust to outliers in point correspondences between image pairs, and a convex program to maintain robustness to outlier directions. In the presence of partially corrupted measurements, we empirically demonstrate that our convex formulation can even recover the locations exactly. Lastly, we demonstrate the utility of our formulations through experiments on Internet photo collections.

(Joint work with Amit Singer.)

22. Thu 28 July, 4:20-5pm

Martin Vetterli, *EPFL, Switzerland*

Euclid's SLAM[12] dunk

Positioning has been around since the dawn of civilization, from recovering landownership after floods in ancient Egypt or the longitude competition for seafaring in 18th century England, to the ubiquity of GPS today. Positioning dovetails with mapping, again a venture pursued for millennia. Doing the two at the same time is much more recent, and famously epitomized in the SLAM problem. Initially conceived as a modality-generic computational method, modern SLAM use cases are in computer vision and time of flight (ToF) positioning with light, radio, or sound. With ToFs we get distances from which we can reason about the trajectory and the environment. Thus a fundamental object related to localization and mapping with ToF measurements is the Euclidean distance matrix (EDM). In our work, we consider variations on the theme of EDMs in localization and mapping. The twist is that our ToFs come from echoes which puts forward various challenges. For example, ToFs are not labeled—we do not a priori know which reflector generates which echo.

There are many ways to formulate and address SLAM from echoes. We focus on what we believe is the most general and most challenging setting: a single omni-directional source and a single omni-directional receiver. This, too, can come in many tastes and colors. In this talk I will present results for the case when the source is static and the receiver moves, and for the case when colocated source and receiver move together. The latter abstracts into a new problem similar to metric multidimensional unfolding. The difference is that instead of distances between two point sets, we get distances between a point set and a set of halfspaces. This leads to a new class of invariances and new algorithms.

(Joint work with Ivan Dokmanic and Miranda Krekovic.)

23. Fri 29 July, 9-9:30

Georgina Hall, *Princeton University, USA*

Polynomial DC Decompositions and Applications

Difference of Convex (DC) programing is a class of optimization problems where the objective and constraints are given as the difference of two convex functions. Although several important problems (e.g., in machine learning) already appear in DC form, such a decomposition is not always available. We consider this decomposition question for polynomial optimization and present algorithms based on linear, second order cone, or semidefinite programming that can find so-called undominated DC decompositions. We also present applications to distance geometry problems.

[12] Simultaneous Localization And Mapping.

24. Fri 29 July, 9:30-10

Yuehaw Khoo, *Princeton University, USA*

Integrating NOE and RDC using Semidefinite Programming for Protein Structure Determination

Nuclear magnetic resonance (NMR) spectroscopy is the most-used technique for protein structure determination besides X-ray crystallography. Typically the 3D structure of a protein is obtained through finding the coordinates of atoms subject to pairwise distance constraints. However, for large proteins there are usually insufficient distance measurements and the structure determination problem becomes ill-posed. Residual dipolar coupling (RDC) measurements provide additional geometric information on the angles between bond directions and the principal-axis-frame. The optimization problem involving RDC is non-convex and we present a novel convex programming relaxation to it. In simulations we attain the Cramer-Rao lower bound with relatively efficient running time. From real data, we obtain the protein backbone structure for ubiquitin with one Angstrom resolution.

(Joint work with Amit Singer and David Cowburn.)

25. Fri 29 July, 10:30-11:10

Meera Sitharam, *University of Florida at Gainesville, USA*

Efficient Realization of Linkages via Optimal Recursive Decomposition, Rigidity, and Cayley Convexification

Finding all realizations of distance constraint systems (linkages) is essential for many applications and is a computationally difficult problem already in 2 and 3 dimensions.

(1) As an essential step towards tractability, in the case where the underlying graph is generically independent in the rigidity matroid, we formalize the notion of a canonical recursive decomposition of an input graph into its (proper) maximal rigid subgraphs, and give a polynomial time algorithm for finding it. The recursive decomposition is a tree with the leaves being edges and the internal nodes being rigid subgraphs (or linkages). The decomposition is optimal in that it minimizes the maximum fanin, which accurately captures the algebraic complexity of the realization problem. The formalization of canonical decomposition, and its optimality extend to general abstract rigidity matroids, and the polynomial time algorithm extends to sparsity matroids.

(2) The realization of a parent linkage in the decomposition tree is achieved by recombining the realizations of its child linkages, thus the problem now reduces to realizing indecomposable linkages. We suggest a new method of optimal modification by dropping edges so that the resulting flexible linkage has a convex, so-called Cayley or nonedge parameterized realization space and moreover, adding in the Cayley nonedges as edges gives a decomposable graph. The convexity and decomposability vastly simplify the search for the required distances of the dropped edges and thus the realizations of the original graph.

While the question of dropping the minimum number of edges (and thus minimizing the dimension of the search space) appears to be NP-hard, we formalize a different optimality condition that ensures an efficient and stable search for realizations.

(3) If time permits, a very brief glimpse of highly related new results by the speaker and coauthors will be provided. (Related to (1)) a newly formulated abstract rigidity matroid called GEM (graded exchange matroid) that will combinatorially capture the 3D rigidity matroid, IF a well-known maximality conjecture is true. (Related to (1)) a new type of rigidity related to incidence geometry that give bounds and algorithms for dictionary learning (Related to (2)): the close connection between the concept of convex Cayley realization spaces and graph flattenability (introduced for the Euclidean norm by Barvinok and studied by Belk/Connelly) in any norm. And finally (Related to (2)): videos demoing opensource software of Cayley realization spaces for molecular assembly and CAD applications.

26. Fri 29 July, 11:10-11:50

Abdo Al-Fakih, *University of Windsor, Canada*

On the uniqueness of the EDM Completion problem, also known as the bar framework universal rigidity problem

An $n \times n$ matrix $D = (d_{ij})$ is called a *Euclidean distance matrix* (*EDM*) if there exist points $p^1, \ldots, p^n$ in some Euclidean space such that $d_{ij} = ||p^i - p^j||^2$ for all $i, j \in \{1, \ldots, n\}$. Given a partial matrix A where some of its entries are specified or fixed and the others are unspecified or free, the *EDM Completion problem* is the problem of completing A into an EDM by assigning values to its free entries.

In this talk, we are interested in the uniqueness of a given EDM completion of A. This problem is also known as the bar framework universal rigidity problem. In particular, we are interested in a sufficient condition for a given free entry of A to assume the same value in all EDM completions of A. Obviously, such condition leads into a sufficient condition for the uniqueness of a given EDM completion of A.

27. Fri 29 July, 2:20pm-3:00pm

Antony Man-Cho So, *Chinese University of Hong Kong*

Robust Convex Approximation Methods for TDOA-Based Localization under NLOS Conditions

In this talk, we present a novel robust optimization approach to source localization using time-difference-of-arrival (TDOA) measurements that are collected under non-line-of-sight (NLOS) conditions. A key feature of our approach is that it does not require knowledge of the distribution or statistics of the NLOS errors, which are often difficult to obtain in practice. Instead, it only assumes that the NLOS errors have bounded supports. Based on this assumption, we formulate the TDOA-based source localization problem as a robust least squares (RLS) problem, in which a location estimate that is robust against the NLOS errors is sought. Since the RLS problem is non-convex, we propose two efficiently implementable convex relaxation-based approximation methods to tackle it. We then analyze the approximation quality of these two methods and establish conditions under which they will yield a unique localization of the source.

28. Fri 29 July, 3:00pm-3:30pm

Shin-Ichi Tanigawa, *Kyoto University, Japan*

Singularity Degree of the Positive Semidefinite Matrix Completion Problem

The singularity degree of a semidefinite programming problem is the smallest number of facial reduction steps to make the problem strongly feasible. We introduce two new graph parameters, called the singularity degree and the nondegenerate singularity degree, based on the singularity degree of the positive semidefinite matrix completion problem. We give a characterization of the class of graphs whose parameter value is equal to one for each parameter. Specifically, we show that the singularity degree of a graph is equal to one if and only if the graph is chordal, and the nondegenerate singularity degree of a graph is equal to one if and only if the graph is the clique sum of chordal graphs and K4-minor free graphs. We also show that the singularity degree is bounded by two if the treewidth is bounded by two, and exhibit a family of graphs with treewidth three, whose singularity degree grows linearly in the number of vertices.

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