DIMACS Workshop on

Optimization in Distance Geometry

26-28 June 2019 at DIMACS, Rutgers University, NJ

Organization

Tami Carpenter, *DIMACS, Rutgers University, USA*
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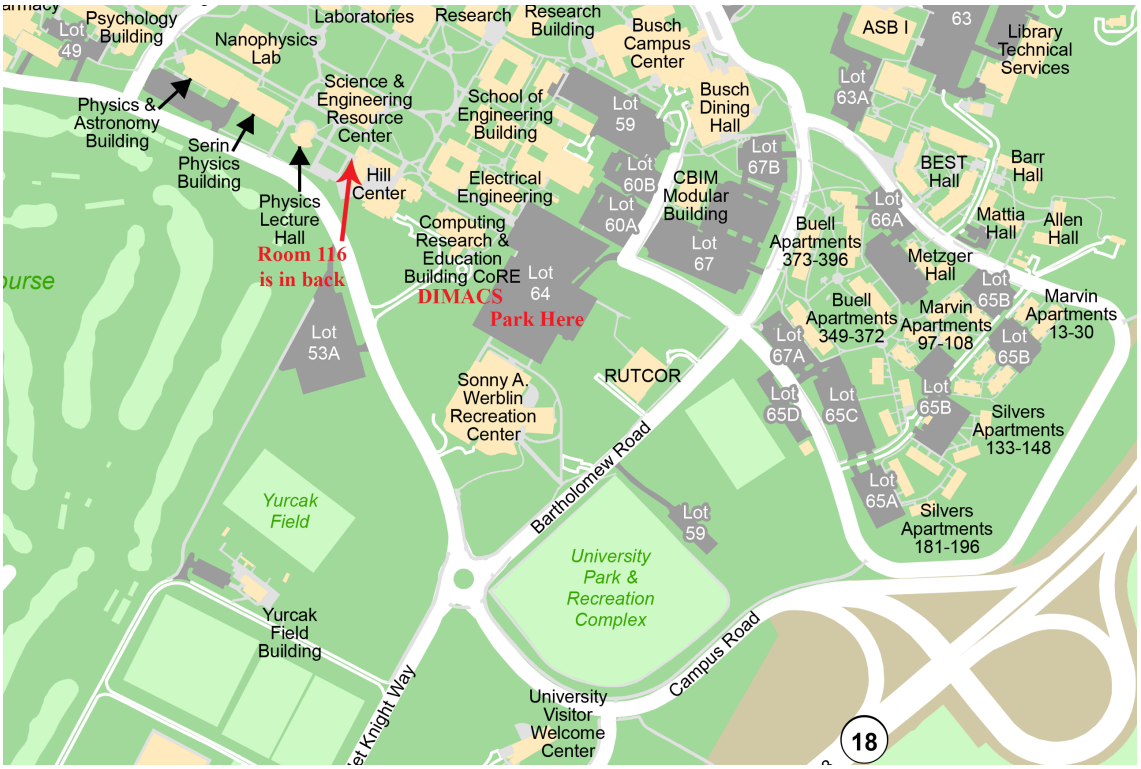
Timetable

	Wed Jun 26	Thu Jun 27	Fri Jun 28
	DIMACS CoRE Building	Room 116 Hill Center	DIMACS CoRE Building
08:30 – 08:50 08:50 – 09:00	Breakfast / Reg. Welcome	Breakfast / Reg.	Breakfast / Reg.
09:00 – 09:40 09:40 – 10:20	Alfakih (Tutorial)	Duxbury (Tutorial)	Streinu (Tutorial)
10:20 – 10:40	Break	Break	Break
10:40 – 11:20 11:20 – 12:00	Tasissa Baez	Lin Souza	Nixon Dümbgen
12:00 – 13:20	Lunch	Lunch	Lunch
13:20 – 14:00 14:00 – 14:40	Liberti (Tutorial)	Omer Maculan	Freitas Vidal
14:40 – 15:00	Break	Break	Closing
15:00 – 15:40 15:40 – 16:20 16:20 – 17:00	Wolkowicz Ahmadi Khoo	Singer Huang Leduino	
17:00 – 18:30			
18:30 – 20:00		Dinner at Panico's 94 Church Street	



2019 DIMACS Workshop on Optimization in Distance Geometry

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Distance Geometry (DG) is a consolidated research area bridging mathematics and computer science [6, 8]. Several real-life applications can be formulated as DG problems. There are a few "classical" applications of DG, including protein conformation determination [3] in structural biology, and sensor network localization [2]. However, new emerging applications have found suitable DG formulations (see, for example, [1, 7]).

DG basically asks whether a simple weighted undirected graph G can be embedded in a given space so that the distances, associated to the edges of G, are realized by the vertex positions [6]. Although the natural formulation of DG is as a constraint satisfaction problem, most DG solution methods are based on a formulation as an optimization problem. Depending on the instance at hand, a semidefinite programming (SDP) formulation can be supplied [4], or a combinatorial formulation [5], just to cite two examples.

Throughout the last few years, the DG community has been organizing regular meetings in order to exchange ideas and experiences on the different facets of the topic. The very first workshop[1] was named "Distance Geometry and Applications" and held in Manaus (Amazonas, Brazil) in 2013. This initial workshop was then followed in 2014 by the workshop[2] "Many Faces of Distances", that was held in Campinas (São Paulo, Brazil). These two initial events already focused on the high multidisciplinary nature of the topic, with particular attention to several applications of DG, as well as to its various and different facets. Among the various disciplines of DG, we can include mathematics, computer science, and optimization, while its applications can arise in biology, chemistry, physics, robotics, virtual reality, recommender systems, human movement simulations, and so on.

In 2016, two events took place. One event,[3] named "Distance Geometry: Theory and Applications," was held here at the DIMACS center of Rutgers University. While this first workshop in 2016 gave emphasis to both theory and applications of DG, the second event[4] of the year (the "Distance Geometry Day", held in Rennes, France) was particularly focused on the applications, including some new applications that were presented by researchers who had, at the time the event took place, only a slight idea of what DG was.

[1] http://dga2013.icomp.ufam.edu.br/
[2] https://www.ime.unicamp.br/workshop_distances/
[3] http://archive.dimacs.rutgers.edu/Workshops/Distance/
[4] https://www.antoniomucherino.it/events/DGD16/

In 2017, the workshop "Distance Geometry" was organized in Bad Honnef[5], Germany, with a focus on inverse problems and optimization. In 2018, the workshop "NMR Protein Determination: Theory and Methods" was held in Campinas (São Paulo, Brazil), where the focus was mainly given to applications in the field of structural biology. In this very last workshop (chronologically), a new format was used where presentations were scheduled on 90 minute-long time slots, and where participants were strongly encouraged to interrupt the speakers to ask any questions they had. This workshop was probably the one that counted the largest number of discussions among the participants.

For all workshops listed above, the scientific programs were defined by the corresponding scientific committees in an invitation-based fashion. Only in a few cases, the presentation of scientific works was open to the entire community (non-invited abstracts were, for example, collected for the workshop in Manaus in 2013, and they were presented in a poster session). It is in fact our feeling that, for all these DG events, the intent of the organizers is mostly to bring together researchers and practitioners having different backgrounds but with potential overlapping research interests. This is particularly evident when researchers working on some of the DG applications are invited to the events, even when their previous knowledge about DG is very little.

The present workshop, held at the DIMACS center in June 2019, has as main aim to continue this tradition of DG-related events. Our main focus this year is on DG approaches which lead to the formulation of an optimization problem, with the idea to construct and consolidate a bridge between DG and optimization. This book of abstracts presents, in a synthetic way, the content of the different research contributions. All invited speakers, moreover, will be invited to contribute with a research article detailing their work to a special issue of Journal of Global Optimization (JOGO, Springer), that we will be editing after the workshop.

We are glad to contribute to this chain of events about DG and its applications with this workshop at the DIMACS center. A lot of new scientific discoveries came out of the previous workshops, and we like to imagine that part of this success is due to these regular events that bring together people to begin new and fruitful collaborations.

Piscataway (NJ), June 2019

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[5] `http://www.lix.polytechnique.fr/~liberti/dg17/index.html`

References

[1] S. Billinge, P. Duxbury, D. Gonçalves, C. Lavor, A. Mucherino, *Recent Results on Assigned and Unassigned Distance Geometry with Applications to Protein Molecules and Nanostructures*, Annals of Operations Research **271**, 161-203, 2018.

[2] P. Biswas, T. Lian, T. Wang, Y. Ye, *Semidefinite Programming based Algorithms for Sensor Network Localization*, ACM Transactions in Sensor Networks **2**, 188–220, 2006.

[3] G.M. Crippen, T.F. Havel, *Distance Geometry and Molecular Conformation*, John Wiley & Sons, 1988.

[4] N. Krislock, H. Wolkowicz, *Explicit Sensor Network Localization using Semidefinite Representations and Facial Reductions*, SIAM Journal on Optimization **20**, 2679–2708, 2010.

[5] C. Lavor, L. Liberti, N. Maculan, A. Mucherino, *The Discretizable Molecular Distance Geometry Problem*, Computational Optimization and Applications **52**, 115–146, 2012.

[6] L. Liberti, C. Lavor, N. Maculan, A. Mucherino, *Euclidean Distance Geometry and Applications*, SIAM Review **56**, 3–69, 2014.

[7] A. Mucherino, C. Lavor (Eds.), *Applications of Distance Geometry*, special issue of Optimization Letters, Springer, 2020.

[8] A. Mucherino, C. Lavor, L. Liberti, N. Maculan (Eds.), *Distance Geometry: Theory, Methods and Applications*, Springer, 329–350, 2013.

Abstracts

1. Wed Jun 26, 09:00 – 10:20

Abdo Alfakih, *University of Windsor, Canada*

On Euclidean Distance Matrices and Spherical Configurations (*tutorial*)

An n-by-n matrix D is a *Euclidean distance matrix (EDM)* if its entries can be realized as the interpoint squared Euclidean distances of an n-point configuration. If the points of the configuration lie on a sphere of radius ρ, then the corresponding EDM is said to be *spherical* of radius ρ.

In the first part of this talk, I will survey the basic theory of EDMs, where the main emphasis will be on various properties and characterizations of EDMs and spherical EDMs. In the second part, I will discuss recently obtained results on a couple of distance geometry problems posed in terms of EDMs. The following is an example of such problems. Given a spherical EDM D of unit radius and $1 \leq k < l \leq n$, characterize the set of all spherical EDMs of unit radius whose entries agree with those of D except possibly with the entry in the klth and lkth positions.

2. Wed Jun 26, 10:40 – 11:20

Abiy Tasissa, *Rensselaer Polytechnic Institute (RPI), USA*

A Matrix Completion Framework for the Euclidean Distance Geometry Problem

The Euclidean distance geometry (EDG) problem naturally arises in a wide variety of applications ranging from determining molecular conformations in computational chemistry to localization in sensor networks. We formulate the EDG problem as a matrix completion problem of recovering a low rank r Gram matrix with respect to certain predefined basis. The well known restricted isometry property can not apply to this formulation. Instead, we introduce a dual basis approach to theoretically analyze the proposed program. If the Gram matrix satisfies certain coherence condition, our main result shows that the underlying configuration of n points can be recovered with high probability from $O(nr \log^2 n)$ uniformly random samples of the distance matrix. Computationally, simple and fast algorithms are designed to solve the Euclidean distance geometry problem. Numerical tests on different three dimensional data and protein molecules validate effectiveness and efficiency of the proposed algorithms.

3. Wed Jun 26, 11:20 – 12:00

Andres David Baez, *Federal University of Technology – Paraná, Brazil*

A Method for Estimation of Unknown Distances in a Class of Euclidean Distance Matrix Completion Problems with Interval Data

We consider some Euclidean distance matrix (EDM) completion problems, inspired by molecular determination problems. Some distances in the matrix are precisely known, some distances are given in terms of intervals and some distances are completely unknown. We propose a method for estimation of the values of the unknown distances in the matrix, based on results about minimal rank EDM completions.

4. Wed Jun 26, 13:20 – 14:40

Leo Liberti, *Centre national de la recherche scientifique (CNRS) and École Polytechnique, France*

Distance Geometry in Data Science (*tutorial*)

Many problems in data science are addressed by mapping entities of various kind to vectors in a Euclidean space of some dimension. Most of these methods (e.g. Multidimensional Scaling, Principal Component Analysis, K-means clustering, random projections) are based on the proximity of pairs of vectors. In order for the results of these methods to make sense, the proximity of entities in the original problem must be well approximated in the Euclidean space setting. If proximity were known for each pair of original entities, this mapping would be a good example of isometric embedding. Usually, however, this is not the case, as data are partial, noisy and wrong. I shall survey some of the methods above from the point of view of Distance Geometry.

5. Wed Jun 26, 15:00 – 15:40

Henry Wolkowicz, *University of Waterloo, Canada*

Completions for Special Classes of Matrices: Euclidean Distance, Low Rank, Sparse, and Toeplitz

We consider the matrix completion problem for special classes of matrices. This includes EDM, low rank, robust PCA, and Toeplitz. We consider both the exact and noisy cases. We include theoretical results as well as efficient numerical techniques. Our tools are semidefinite programming, facial reduction, and trust region subprob-

lems.

6. Wed Jun 26, 15:40 – 16:20

Amir Ali Ahmadi, *Princeton University, USA*

Time-Varying Semidefinite Programs

We study time-varying semidefinite programs (TV-SDPs), which are semidefinite programs whose data (and solutions) are functions of time. Our focus is on the setting where the data varies polynomially with time. We show that under a strict feasibility assumption, restricting the solutions to also be polynomial functions of time does not change the optimal value of the TV-SDP. Moreover, by using a Positivstellensatz on univariate polynomial matrices, we show that the best polynomial solution of a given degree to a TV-SDP can be found by solving a semidefinite program of tractable size. We also provide a sequence of dual problems which can be cast as SDPs and that give upper bounds on the optimal value of a TV-SDP (in maximization form). We prove that under a boundedness assumption, this sequence of upper bounds converges to the optimal value of the TV-SDP. Under the same assumption, we also show that the optimal value of the TV-SDP is attained. We demonstrate the efficacy of our algorithms on a maximum-flow problem with time-varying edge capacities, a wireless coverage problem with time-varying coverage requirements, and on bi-objective semidefinite optimization where the goal is to approximate the Pareto curve in one shot. Joint work with Bachir El Khadir (Princeton).

7. Wed Jun 26, 16:20 – 17:00

Yuehaw Khoo, *Stanford University, USA*

Clique-Based Semidefinite Relaxation of the Quadratic Assignment Problem

The matching problem between two adjacency matrices, A and B, can be formulated as the NP-hard quadratic assignment problem (QAP). While the QAP admits a semidefinite (SDP) relaxation that is often tight in practice, this SDP scales badly as it involves a matrix variable of size n^2 by n^2. To achieve a speed up, a further relaxation of the SDP will be described, where the number of variables scale as $O(bn^2)$, where b is the number of non-zero entries in B. The dual problem of this relaxation has a natural three-block structure that can be solved via Alternating Direction Method of Multipliers (ADMM) in a distributed manner. I will show results that suggest this relaxation offers a good compromise between speed and tightness in practice, and will discuss how the assignment problem in Nuclear Magnetic Resonance Spectroscopy can be formulated as a QAP with sparse B. This is joint work with Jose Simoes Bravo

Ferreira and Amit Singer.

8. Thu Jun 27, 09:00 – 10:20

Phillip M. Duxbury, *Michigan State University, USA*

Unassigned Distance Geometry, Graph Rigidity and the Nanostructure Problem (*tutorial*)

This talk will be a tutorial introduction to the unassigned variant (called uDG) of the DG problem, and how it arises in the problem of finding the atomic structure of materials. Two classes of optimization algorithm will be described, with both based on build-up methods but using different strategies. Classes of problem for which the buildup methods are exact will be outlined and bounds on their computational time will be derived and tested using computational experiments. As in the DG problem, graph rigidity provides useful insights into the minimal number of distances that are required for there to be a unique solution to the uDG problem. A list of unsolved problems in the area will be discussed.

9. Thu Jun 27, 10:40 – 11:20

Jung-Hsin Lin, *Academia Sinica, Taiwan*

Protein Conformation Evolution with a Branch-and-Prune Algorithm for Discretizable Distance Geometry Problems

Conformational sampling for biological macromolecules, e.g., proteins, DNA, RNA, etc., usually relies on molecular dynamics simulations (MDS), either in explicit solvent or with continuum electrostatic models to mimic the physiological environment of the biomolecules. MDS are intrinsically an N-particle move conformational sampling algorithm, in which the movement of each atom is guided by the force experienced. To avoid steric collision, the movement for each step has to be small so that MDS can be conducted smoothly. MDS usually will be terminated if the system evolves into bad configurations. Another popular sampling approach is the Monte Carlo method, and the Metropolis algorithm is commonly applied if the canonical ensemble distribution is desired. Monte Carlo methods have the advantages of being more robust, and can be conducted with bad initial configuration. However, there is no efficient N-particle move algorithm for the Monte Carlo sampling of biomolecular conformations, if the force calculations are to be avoided. We recently proposed a new method to construct the protein conformations by solving the discretizable distance geometry problem with interval data, and we now apply this method to generate the conformations for the Monte Carlo move of the protein conformations. We will demonstrate the efficiency of sampling of our method with various sampling strategies for folded protein structures,

and also test whether our method could be suitable protein folding simulations. Joint work with Antonio Mucherino, IRISA, University of Rennes 1, France.

10. Thu Jun 27, 11:20 – 12:00

Michael Souza, *Federal University of Ceará, Brazil*

Advances and New Challenges on Branch-and-Prune Algorithm

The Branch-and-Prune algorithm (BP) and its variations are among the most cited methods to solve molecular discretizable distance geometry problems (DMDGP). The BP-like algorithms represent the DMDGP by a graph whose nodes are ordered in such a way that a solution can be constructed iteratively. Previous results indicated that finding a BP-order was a NP-hard problem, but in this presentation we show that it can be done in polynomial time. An interesting property of DMDGP is that all solutions can be generated from any other applying partial reflections. We also introduce a new application of this result using it to reduce the number of float point operations required by BP to calculate a solution to DMDGP. Finally, we define a NP-hard problem whose solution identifies the minimal number operations needed to solve the DMDGP with BP algorithm.

11. Thu Jun 27, 13:20 – 14:00

Jeremy Omer, *Institut National des Sciences Appliquées (INSA) de Rennes, France*

Discretization of Distance Geometry Graphs: Algorithmic Complexity and Solution Methods

Discretizable distance geometry problems (DDGPs) constitute a class of graph realization problems where the vertices can be ordered in such a way that the search space of possible positions becomes discrete, usually represented by a binary tree. In dimension K, a discretization order is such that each one of the vertices with rank greater than $K+1$ has at least K adjacent predecessors, called references. Finding such vertex orders is an essential step to identify and solve DDGPs. Here we look for discretization orders that minimize one of two distinct indicators of the size of the search tree. With both indicators, the key is to have a small number of vertices with exactly K references. In the first part of the presentation, we will consider a generalization of this discretization problem and show that it is strongly NP-Hard with both indicators, even if K is fixed to any value larger than or equal to one. In the second part, I will talk about two different solution methods for this problem. One is a cutting plane algorithm based on an extended integer programming formulation. The other is a branch-and-bound algorithm making use of a previously developed greedy

algorithm that is guaranteed to return a discretization order when one exists. Finally, I will discuss a numerical comparison of the different approaches on a benchmark based on distance geometry instances.

12. Thu Jun 27, 14:00 – 14:40

Nelson Maculan, *Federal University of Rio de Janeiro, Brazil* & Hacene Ouzia, *Sorbonne University, France*

Mixed Integer Nonlinear Optimization Models for the Euclidean Steiner Tree Problem in $\mathbb{R}^d$

New mixed integer nonlinear optimization models for the Euclidean Steiner tree problem in d-space (with $d \geq 3$) will be presented in this talk. Each model features a non smooth objective function but a convex set of feasible solutions. All these models are theoretically equivalent. From these models, six mixed integer linear and nonlinear relaxations will be considered. Each relaxation has the same set of feasible solutions as the model from which it is derived. Finally, preliminary computational results highlighting the main features of the presented relaxations will be discussed.

13. Thu Jun 27, 15:00 – 15:40

Amit Singer, *Princeton University, USA*

Autocorrelation Analysis in Cryo-Electron Microscopy

Autocorrelation analysis offers an alternative computational framework for 3-D structure determination of biological macromolecules using single particle cryo-EM. Similar to distance geometry, autocorrelation analysis also requires solving a system of low degree polynomial equations and the question of uniqueness plays a significant role.

14. Thu Jun 27, 15:40 – 16:20

Shuai Huang, *University of Illinois Urbana-Champaign, USA*

Computational Cryo-electron Microscopy via Unassigned Distance Geometry

Cryo-electron microscopy (cryo-EM) tries to reconstruct a 3D molecule structure from a collection of random 2D projections with unknown view angles. Previous approaches formulate the reconstruction as a maximum likelihood problem, and solve it using methods such as expectation maximization whose performance often

depends on the initialization. In this talk, starting from a 3D point-source model, we reveal the connection between cryo-EM and the unassigned distance geometry problem (uDGP), and show that unlabelled pairwise and radial distances could be extracted from random 2D projections. We can express the unlabelled pairwise and radial distances as quadratic and linear measurements of the 3D point-source model respectively, and recast the reconstruction into a constrained nonconvex optimization problem. This way we can construct a suitable initializer via a modified spectral initialization strategy and solve it using projected gradient descent. We next extend the proposed approach to the more general 3D Gaussian-source model, and highlight the differences and challenges in the corresponding optimization problem.

15. Thu Jun 27, 16:20 – 17:00

Luiz Leduino, *Federal University of Sao Paolo, Brazil*

Solving the Unassigned Distance Geometry Problem via Nonlinear Programming

We propose new mathematical programming formulations and a new heuristic to solve the unassigned distance geometry problem. Preliminary computational results are also presented.

16. Fri Jun 28, 09:00 – 10:20

Ileana Streinu, *Smith College, USA*

Structure in Motion (*tutorial*)

I will present a tutorial on rigidity theory for bar-and-joint frameworks with a focus on flexible structures, both finite and periodic. I will cover generic properties captured by combinatorial descriptors, infinitesimal and continuous deformations, and how to design flexible structures with special kinds of trajectories, such as those that avoid singularities, expand all distances or, in crystals, just the unit cells. Along the way, applications in robotics, structural molecular biology and materials science will be described. This is a summary of a joint project with Ciprian Borcea, supported by a 2018-19 fellowship at Harvards Radcliffe Institute for Advanced Study.

17. Fri Jun 28, 10:40 – 11:20

Anthony Nixon, *Lancaster University, UK*

Global Rigidity of Linearly Constrained Frameworks

A (bar-joint) framework (G, p) in $\mathbb{R}^d$ is the combination of a graph G and a map p assigning positions to the vertices of G. A framework is rigid if the only edge-length-preserving continuous motions of the vertices arise from isometries of $\mathbb{R}^d$. The framework is globally rigid if every other framework with the same edge lengths arises from isometries of $\mathbb{R}^d$. Both rigidity and global rigidity, generically, are well understood when $d = 2$.

A linearly constrained framework in $\mathbb{R}^d$ is a generalisation of a framework in which some vertices are constrained to lie on one or more given hyperplanes. Streinu and Theran characterised rigid linearly constrained generic frameworks in $\mathbb{R}^2$ in 2010. In this talk I will describe an analogous result for the global rigidity of linearly constrained generic frameworks in $\mathbb{R}^2$. This is joint work with Hakan Guler and Bill Jackson.

18. Fri Jun 28, 11:20 – 12:00

Frederike Dümbgen, *École Polytechnique Fédérale de Lausanne (EPFL), Switzerland*

Towards Hybrid Indoor Localization Using Range and Direction Measurements

Humans use a wealth of heterogeneous signals to navigate through space. We leverage the rich visual signals from our retina, combine it with acoustic and inertial measurements from the auditory system, tactile signals, and others, to sense our surroundings. We learn to travel efficiently through an environment, to reorient ourselves when we get lost, and to create cognitive maps for future use. The diversity of signals improves the accuracy of our navigation, and it provides us with a resilience to failure of different pieces of sensory information.

Inspired by this, we develop an indoor localization system which can provide accurate localization by aggregating signals from different modalities. In this talk, I will provide both theoretical and practical insights which can pave the way for such a multimodal system. From a theoretical viewpoint, I will present our research on combining range and direction measurements in a sensor localization setting using a new algebraic framework called Coordinate Difference Matrices. Then, I will switch to a more practical setting and present our real-time localization algorithm using a Conditional Random Field to include measurements of different types in a probabilistic way. Results from indoor localization experiments using Bluetooth, WiFi, inertial measurement units and visual measurements validate the good performance of this framework even for signals with high bias and variance.

This work is done in collaboration with other members of the laboratory of audiovisual communications (LCAV), the school of engineering and architecture of Fribourg (HEIA-FR), and Vidinoti.

19. Fri Jun 28, 13:20 – 14:00

Rosiane Freitas, *Federal University of Amazonas, Brazil*

Distance Coloring Graph Problems: Theoretical Models, Methods and Applications

Graph coloring constitutes a class of combinatorial optimization problems of great theoretical and practical relevance with many applications, for which variations have been proposed in the literature, using different characteristics applied to vertices and edges. One of its most important applications is the channel assignment in mobile wireless networks, where channels must be attributed to devices while avoiding interferences, for which the Bandwidth Coloring Problem (BCP) has been proposed, where colors assigned to vertices must be separated according to weights imposed on edges. However, such a model does not take into account all scenarios of the channel assignment so other theoretical approaches can be used to identify new models. In this talk, we present new coloring problems based on distance geometry, generalizing the classic Vertex Coloring Problem (VCP) and BCP with adjacency constraints involving equalities and inequalities, which can be applied to different characteristics of the channel assignment, such as bidirectional communication. For the new models, we present feasibility and computational complexity properties. We propose constraint programming formulations based on such problem definitions, using global constraints for treating multi-coloring demands. Also, we explored integer programming models for BCP, improving an existing one and proposing two new others, based on orientations of the input graph and distances between colors. Both new models have polynomial size, in contrast to existing ones that are pseudopolynomial. For the new corresponding polytopes, we present their properties and valid inequalities which define facets under certain conditions. We also developed a cut-and-branch algorithm based on the orientation polytope and its valid inequalities. Our experiments show that this strategy has good potential for BCP, obtaining optimal solutions in less runtime when compared to the standard formulation for many literature instances.

20. Fri Jun 28, 14:00 – 14:40

Thibaut Vidal, *Pontifical Catholic University of Rio de Janeiro, Brazil*

Phase Unwrapping and Operations Research

Phase unwrapping is the process of recovering a continuous phase signal from an original signal wrapped in the $]-\pi,\pi]$ interval. It is a critical step of coherent signal processing, with applications such as synthetic aperture radar, acoustic imaging, magnetic resonance, X-ray crystallography, and seismic processing, and thus the subject of extensive research. We reformulate the phase unwrapping problem under $L0$-norm as the search for a minimum-cost balanced spanning forest in a graph where the vertices

represent the residues of the wrapped phase, and introduce branch-and-cut, column generation and metaheuristic approaches. These approaches lead us one step closer towards good solutions for this problem, which were previously viewed, in the signal processing literature, as highly desirable but nonetheless intractable.

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