

Antonio Mucherino · Carlile Lavor
Leo Liberti · Nelson Maculan *Editors*

Distance Geometry

Theory, Methods, and Applications

 Springer

Distance Geometry Theory Methods And Applications

Klaus Müller



Distance Geometry Theory Methods And Applications:

Distance Geometry Antonio Mucherino, Carlile Lavor, Leo Liberti, Nelson Maculan, 2012-12-22 This volume is a collection of research surveys on the Distance Geometry Problem DGP and its applications It will be divided into three parts Theory Methods and Applications Each part will contain at least one survey and several research papers The first part Theory will deal with theoretical aspects of the DGP including a new class of problems and the study of its complexities as well as the relation between DGP and other related topics such as distance matrix theory Euclidean distance matrix completion problem multispherical structure of distance matrices distance geometry and geometric algebra algebraic distance geometry theory visualization of K dimensional structures in the plane graph rigidity and theory of discretizable DGP symmetry and complexity The second part Methods will discuss mathematical and computational properties of methods developed to the problems considered in the first chapter including continuous methods based on Gaussian and hyperbolic smoothing difference of convex functions semidefinite programming branch and bound discrete methods based on branch and prune geometric build up graph rigidity and also heuristics methods based on simulated annealing genetic algorithms tabu search variable neighborhood search Applications will comprise the third part and will consider applications of DGP to NMR structure calculation rational drug design molecular dynamics simulations graph drawing and sensor network localization This volume will be the first edited book on distance geometry and applications The editors are in correspondence with the major contributors to the field of distance geometry including important research centers in molecular biology such as Institut Pasteur in Paris

Open Problems in Optimization and Data Analysis Panos M. Pardalos, Athanasios Migdalas, 2018-12-04 Computational and theoretical open problems in optimization computational geometry data science logistics statistics supply chain modeling and data analysis are examined in this book Each contribution provides the fundamentals needed to fully comprehend the impact of individual problems Current theoretical algorithmic and practical methods used to circumvent each problem are provided to stimulate a new effort towards innovative and efficient solutions Aimed towards graduate students and researchers in mathematics optimization operations research quantitative logistics data analysis and statistics this book provides a broad comprehensive approach to understanding the significance of specific challenging or open problems within each discipline The contributions contained in this book are based on lectures focused on Challenges and Open Problems in Optimization and Data Science presented at the Deucalion Summer Institute for Advanced Studies in Optimization Mathematics and Data Science in August 2016

Geometric Science of Information Frank Nielsen, Frédéric Barbaresco, 2017-10-30 This book constitutes the refereed proceedings of the Third International Conference on Geometric Science of Information GSI 2017 held in Paris France in November 2017 The 101 full papers presented were carefully reviewed and selected from 113 submissions and are organized into the following subjects statistics on non linear data shape space optimal transport and applications image processing optimal transport and applications signal

processing statistical manifold and hessian information geometry monotone embedding in information geometry information structure in neuroscience geometric robotics and tracking geometric mechanics and robotics stochastic geometric mechanics and Lie group thermodynamics probability on Riemannian manifolds divergence geometry non parametric information geometry optimization on manifold computational information geometry probability density estimation session geometry of tensor valued data geodesic methods with constraints applications of distance geometry Dynamics of Information Systems Hossein Moosaei, Milan Hladik, Panos M. Pardalos, 2023-12-27 This book constitutes the proceedings of the 6th International Conference on Dynamics of Information Systems DIS 2023 which took place in Prague Czech Republic in September 2023 The 18 full papers included in the book were carefully reviewed and selected from 43 submissions They deal with topics ranging from theoretical algorithmic and practical perspectives in information systems to offering readers valuable information theories and techniques Euclidean Distance Geometry Leo Liberti, Carlile Lavor, 2017-09-20 This textbook the first of its kind presents the fundamentals of distance geometry theory useful methodologies for obtaining solutions and real world applications Concise proofs are given and step by step algorithms for solving fundamental problems efficiently and precisely are presented in Mathematica enabling the reader to experiment with concepts and methods as they are introduced Descriptive graphics examples and problems accompany the real gems of the text namely the applications in visualization of graphs localization of sensor networks protein conformation from distance data clock synchronization protocols robotics and control of unmanned underwater vehicles to name several Aimed at intermediate undergraduates beginning graduate students researchers and practitioners the reader with a basic knowledge of linear algebra will gain an understanding of the basic theories of distance geometry and why they work in real life **Computational Topology in Image Context** Alexandra Bac, Jean-Luc Mari, 2016-06-01 This book constitutes the proceedings of the 6th International Workshop on Computational Topology in Image Context CTIC 2016 held in Marseille France in June 2016 The 24 papers presented in this volume were carefully reviewed and selected from 35 submissions Additionally this volume contains 2 invited papers CTIC covers a wide range of topics such as topological invariants and their computation homology cohomology linking number fundamental groups algorithm optimization in discrete geometry transfer of mathematical tools parallel computation in multi dimensional volume context hierarchical approaches experimental evaluation of algorithms and heuristics combinatorial or multi resolution models discrete or computational topology geometric modeling guided by topological constraints computational topological dynamics and use of topological information in discrete geometry applications **Simulation of Material Processing: Theory, Methods and Application** Ken-ichiro Mori, 2001-01-01 This volume contains about 180 papers including seven keynotes presented at the 7th NUMIFORM Conference It reflects the state of the art of simulation of industrial forming processes such as rolling forging sheet metal forming injection moulding and casting Theory and Applications of Distance Geometry Leonard Mascot Blumenthal, 1970 Hemispherical

Photography in Forest Science: Theory, Methods, Applications Richard A. Fournier, Ronald J. Hall, 2017-05-11 This book presents practical information about hemispherical photography from the perspectives of field data acquisition image processing and information retrieval methods This book is organized into three sections The first section describes what is hemispherical photography and what are the fundamental elements of forest structure and light interactions within the forest canopy The second section provides practical information about the equipment procedures and tools for procuring processing and analyzing hemispherical photographs Armed with this information the third section describes several applications of hemispherical photographs to forestry and natural resource assessment The book concludes with a discussion about modelling tools and future directions of this rapidly growing field There is currently no information source on the market that has this comprehensive range of topics combined in a single book The book will appeal to academics graduate students natural resource professionals and researchers alike **Theory and applications of distance geometry** ,1970

3D QSAR in Drug Design Hugo Kubinyi, Gerd Folkers, Yvonne Connolly Martin, 1998 **Classical and Three-dimensional QSAR in Agrochemistry** Corwin Hansch, 1995 Discusses the applications of classical QSAR and molecular modeling analysis to the discovery of new agrochemicals Examines hydrophobicity parameters derived from various partitioning systems Includes chapters focusing on the use of three dimensional QSAR analyses such as CoMFA and DISCO Presents information on the use of QSAR to study transport and toxicology of agrochemicals *NMR Methods for Elucidating Macromolecule-ligand Interactions* Robert E. Handschumacher, Ian M. Armitage, 1990 The 4th Symposium was held in New Haven Conn July 1989 The four sessions cover current NMR structural methodology and its application analysis of bioactive peptide conformation macromolecular target recognition and drug macromolecular interactions No index Annotation copyright Book News In De Novo Design Klaus Müller, 1995 *Handbook of Molecular Descriptors, Volume 11* Roberto Todeschini, Viviana Consonni, 2000-12-07 It will be an invaluable guide for all those dealing with bioactive molecules as well as for those aimed to predict physico chemical or environmental properties by models based on molecular descriptors This book is written in such way to be also a powerful didactic tool for researchers BOOK JACKET

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