

Distance Geometry Theory Methods And Applications

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Parallel Coordinates - Alfred Inselberg 2009-08-15

This is one book that can genuinely be said to be straight from the horse's mouth. Written by the originator of the technique, it examines parallel coordinates as the leading methodology for multidimensional visualization. Starting from geometric foundations, this is the first systematic and rigorous exposition of the methodology's mathematical and algorithmic components. It covers, among many others, the visualization of multidimensional lines, minimum distances, planes, hyperplanes, and clusters of "near" planes. The last chapter explains in a non-technical way the methodology's application to visual and automatic data mining. The principles of the latter, along with guidelines, strategies and algorithms are illustrated in detail on real high-dimensional datasets.

Systems, Patterns and Data Engineering with Geometric Calculi - Sebastià Xambó-Descamps 2021-07-16

The intention of this collection agrees with the purposes of the homonymous mini-symposium (MS) at ICIAM-2019, which were to overview the essentials of geometric calculus (GC) formalism, to report on state-of-the-art applications showcasing its advantages and to explore the bearing of GC in novel approaches to deep learning. The first three contributions, which correspond to lectures at the MS, offer perspectives on recent advances in the application GC in the areas of robotics, molecular geometry, and medical imaging. The next three, especially invited, hone the expressiveness of GC in orientation measurements under different metrics, the treatment of contact elements, and the investigation of efficient computational methodologies. The last two, which also correspond to lectures at the MS, deal with two aspects of deep learning: a presentation of a concrete quaternionic convolutional neural network layer for image classification that features contrast invariance and a general overview of automatic learning aimed at steering the development of neural networks whose units process elements of a suitable algebra, such as a geometric algebra. The book fits, broadly speaking, within the realm of mathematical engineering, and consequently, it is intended for a wide spectrum of research profiles. In particular, it should bring inspiration and guidance to those looking for materials and problems that bridge GC with applications of great current interest, including the auspicious field of GC-based deep neural networks.

Distance Geometry - Antonio Mucherino 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.

Drug Design - Kenneth M. Merz, Jr 2010-05-31

Structure-based (SBDD) and ligand-based (LBDD) drug design are extremely important and active areas of research in both the academic and commercial realms. This book provides a complete snapshot of the field of computer-aided drug design and associated experimental approaches. Topics covered include X-ray crystallography, NMR, fragment-based drug design, free energy methods, docking and scoring, linear-scaling quantum calculations, QSAR, pharmacophore methods, computational ADME-Tox, and drug discovery case studies. A variety of authors from academic and commercial institutions all over the world have contributed to this book, which is illustrated with more than 200 images. This is the only book to cover the subject of structure and ligand-based drug design, and it provides the most up-to-date information on a wide range of topics for the practising computational chemist, medicinal chemist, or structural biologist. Professor Kenneth Merz has been selected as the recipient of the 2010 ACS Award for Computers in Chemical & Pharmaceutical Research that recognizes the advances he has made in the use of quantum mechanics to solve biological and drug discovery problems.

Discrete and Computational Geometry and Graphs - Jin Akiyama 2016-11-24

This book constitutes the thoroughly refereed post-conference proceedings of the 18th Japanese Conference on Discrete and Computational Geometry and Graphs, JDCDGG 2015, held in Kyoto, Japan, in September 2015. The total of 25 papers included in this volume was carefully reviewed and selected from 64 submissions. The papers feature advances made in the field of computational geometry and focus on emerging technologies, new methodology and applications, graph theory and dynamics. This proceedings are dedicated to Naoki Katoh on the occasion of his retirement from Kyoto University.

Molecular Similarity in Drug Design - P.M. Dean 2012-12-06

Molecular similarity searching is fast becoming a key tool in organic chemistry. In this book, the editor has brought together an international team of authors, each working at the forefront of this technology, providing a timely and concise overview of current research. The chapters focus principally on those methods which have reached sufficient maturity to be of immediate practical use in molecular design.

Open Problems in Optimization and Data Analysis - Panos M. Pardalos 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.

Invariant Methods in Discrete and Computational Geometry - Neil L. White 2013-03-09

Invariant, or coordinate-free methods provide a natural framework for many geometric questions. Invariant Methods in Discrete and Computational Geometry provides a basic introduction to several aspects of invariant theory, including the supersymmetric algebra, the

Grassmann-Cayler algebra, and Chow forms. It also presents a number of current research papers on invariant theory and its applications to problems in geometry, such as automated theorem proving and computer vision. Audience: Researchers studying mathematics, computers and robotics.

Encyclopedia of Optimization - Christodoulos A. Floudas 2008-09-04
The goal of the Encyclopedia of Optimization is to introduce the reader to a complete set of topics that show the spectrum of research, the richness of ideas, and the breadth of applications that has come from this field. The second edition builds on the success of the former edition with more than 150 completely new entries, designed to ensure that the reference addresses recent areas where optimization theories and techniques have advanced. Particularly heavy attention resulted in health science and transportation, with entries such as "Algorithms for Genomics", "Optimization and Radiotherapy Treatment Design", and "Crew Scheduling".

A Geometric Algebra Invitation to Space-Time Physics, Robotics and Molecular Geometry - Carlile Lavor 2018-07-12

This book offers a gentle introduction to key elements of Geometric Algebra, along with their applications in Physics, Robotics and Molecular Geometry. Major applications covered are the physics of space-time, including Maxwell electromagnetism and the Dirac equation; robotics, including formulations for the forward and inverse kinematics and an overview of the singularity problem for serial robots; and molecular geometry, with 3D-protein structure calculations using NMR data. The book is primarily intended for graduate students and advanced undergraduates in related fields, but can also benefit professionals in search of a pedagogical presentation of these subjects.

Progress in Drug Research / Fortschritte der Arzneimittelforschung / Progrès des Recherches Pharmaceutiques - Vijendra K. Singh 2013-03-13

Volume 45 of "Progress in Drug Research" contains eight reviews and the various indexes which facilitate its use and establish the connection with the previous volumes. The articles in this volume deal with neuro peptides as native immune modulators, with Calmodulin and with effects of cell stimuli and drugs on cellular activation, with recent advances in benzodiazepine receptor binding studies, with the medicinal chemistry and therapeutic potentials of ligands of the histamine H3 receptor, with Serotonin uptake inhibitors, with computer-aided drug design, with natri uretic hormones and with the recent developments in the chemotherapy of osteoporosis. In the 36 years that PDR has existed, the Editor has enjoyed the valuable help and advice of many colleagues. Readers, the authors of the reviews and, last but not least, the reviewers have all contributed greatly to the success of this series. Although the comments received so far have generally been favorable, it is nevertheless necessary to analyze and to reassess the current position and the future direction of such a series of monographs. So far, it has been the Editor's intention to help disseminate information on the vast domain of drug research, and to provide the reader with a tool with which to keep abreast of the latest developments and trends. The reviews in PDR are useful to the nonspecialist, who can obtain an overview of a particular field of drug research in a relatively short time.

Distance Geometry and Molecular Conformation - G. M. Crippen 1988

The Organic Chemistry of Drug Design and Drug Action - Richard B. Silverman 2014-03-29

The Organic Chemistry of Drug Design and Drug Action, Third Edition, represents a unique approach to medicinal chemistry based on physical organic chemical principles and reaction mechanisms that rationalize drug action, which allows reader to extrapolate those core principles and mechanisms to many related classes of drug molecules. This new edition includes updates to all chapters, including new examples and references. It reflects significant changes in the process of drug design over the last decade and preserves the successful approach of the previous editions while including significant changes in format and coverage. This text is designed for undergraduate and graduate students in chemistry studying medicinal chemistry or pharmaceutical chemistry; research chemists and biochemists working in pharmaceutical and biotechnology industries. Updates to all chapters, including new examples and references Chapter 1 (Introduction): Completely rewritten and expanded as an overview of topics discussed in detail throughout the book Chapter 2 (Lead Discovery and Lead Modification): Sections on sources of compounds for screening including library collections, virtual screening, and computational methods, as well as hit-to-lead and scaffold hopping; expanded sections on sources of lead compounds, fragment-based lead discovery, and molecular graphics; and deemphasized solid-phase synthesis and

combinatorial chemistry Chapter 3 (Receptors): Drug-receptor interactions, cation- π and halogen bonding; atropisomers; case history of the insomnia drug suvorexant Chapter 4 (Enzymes): Expanded sections on enzyme catalysis in drug discovery and enzyme synthesis Chapter 5 (Enzyme Inhibition and Inactivation): New case histories: for competitive inhibition, the epidermal growth factor receptor tyrosine kinase inhibitor, erlotinib and Abelson kinase inhibitor, imatinib for transition state analogue inhibition, the purine nucleoside phosphorylase inhibitors, forodesine and DADMe-ImmH, as well as the mechanism of the multisubstrate analog inhibitor isoniazid for slow, tight-binding inhibition, the dipeptidyl peptidase-4 inhibitor, saxagliptin Chapter 7 (Drug Resistance and Drug Synergism): This new chapter includes topics taken from two chapters in the previous edition, with many new examples Chapter 8 (Drug Metabolism): Discussions of toxicophores and reactive metabolites Chapter 9 (Prodrugs and Drug Delivery Systems): Discussion of antibody-drug conjugates

Convex Optimization & Euclidean Distance Geometry - Jon Dattorro 2005

The study of Euclidean distance matrices (EDMs) fundamentally asks what can be known geometrically given only distance information between points in Euclidean space. Each point may represent simply location or, abstractly, any entity expressible as a vector in finite-dimensional Euclidean space. The answer to the question posed is that very much can be known about the points; the mathematics of this combined study of geometry and optimization is rich and deep. Throughout we cite beacons of historical accomplishment. The application of EDMs has already proven invaluable in discerning biological molecular conformation. The emerging practice of localization in wireless sensor networks, the global positioning system (GPS), and distance-based pattern recognition will certainly simplify and benefit from this theory. We study the pervasive convex Euclidean bodies and their various representations. In particular, we make convex polyhedra, cones, and dual cones more visceral through illustration, and we study the geometric relation of polyhedral cones to nonorthogonal bases biorthogonal expansion. We explain conversion between halfspace- and vertex-descriptions of convex cones, we provide formulae for determining dual cones, and we show how classic alternative systems of linear inequalities or linear matrix inequalities and optimality conditions can be explained by generalized inequalities in terms of convex cones and their duals. The conic analogue to linear independence, called conic independence, is introduced as a new tool in the study of classical cone theory; the logical next step in the progression: linear, affine, conic. Any convex optimization problem has geometric interpretation. This is a powerful attraction: the ability to visualize geometry of an optimization problem. We provide tools to make visualization easier. The concept of faces, extreme points, and extreme directions of convex Euclidean bodies is explained here, crucial to understanding convex optimization. The convex cone of positive semidefinite matrices, in particular, is studied in depth. We mathematically interpret, for example, its inverse image under affine transformation, and we explain how higher-rank subsets of its boundary united with its interior are convex. The Chapter on "Geometry of convex functions", observes analogies between convex sets and functions: The set of all vector-valued convex functions is a closed convex cone. Included among the examples in this chapter, we show how the real affine function relates to convex functions as the hyperplane relates to convex sets. Here, also, pertinent results for multidimensional convex functions are presented that are largely ignored in the literature; tricks and tips for determining their convexity and discerning their geometry, particularly with regard to matrix calculus which remains largely unsystematized when compared with the traditional practice of ordinary calculus. Consequently, we collect some results of matrix differentiation in the appendices. The Euclidean distance matrix (EDM) is studied, its properties and relationship to both positive semidefinite and Gram matrices. We relate the EDM to the four classical axioms of the Euclidean metric; thereby, observing the existence of an infinity of axioms of the Euclidean metric beyond the triangle inequality. We proceed by deriving the fifth Euclidean axiom and then explain why furthering this endeavor is inefficient because the ensuing criteria (while describing polyhedra) grow linearly in complexity and number. Some geometrical problems solvable via EDMs, EDM problems posed as convex optimization, and methods of solution are presented; e.g., we generate a recognizable isotonic map of the United States using only comparative distance information (no distance information, only distance inequalities). We offer a new proof of the classic Schoenberg criterion, that determines whether a candidate

matrix is an EDM. Our proof relies on fundamental geometry; assuming, any EDM must correspond to a list of points contained in some polyhedron (possibly at its vertices) and vice versa. It is not widely known that the Schoenberg criterion implies nonnegativity of the EDM entries; proved here. We characterize the eigenvalues of an EDM matrix and then devise a polyhedral cone required for determining membership of a candidate matrix (in Cayley-Menger form) to the convex cone of Euclidean distance matrices (EDM cone); i.e., a candidate is an EDM if and only if its eigenspectrum belongs to a spectral cone for EDM^N . We will see spectral cones are not unique. In the chapter "EDM cone", we explain the geometric relationship between the EDM cone, two positive semidefinite cones, and the ellipsope. We illustrate geometric requirements, in particular, for projection of a candidate matrix on a positive semidefinite cone that establish its membership to the EDM cone. The faces of the EDM cone are described, but still open is the question whether all its faces are exposed as they are for the positive semidefinite cone. The classic Schoenberg criterion, relating EDM and positive semidefinite cones, is revealed to be a discretized membership relation (a generalized inequality, a new Farkas-like lemma) between the EDM cone and its ordinary dual. A matrix criterion for membership to the dual EDM cone is derived that is simpler than the Schoenberg criterion. We derive a new concise expression for the EDM cone and its dual involving two subspaces and a positive semidefinite cone. "Semidefinite programming" is reviewed with particular attention to optimality conditions of prototypical primal and dual conic programs, their interplay, and the perturbation method of rank reduction of optimal solutions (extant but not well-known). We show how to solve a ubiquitous platonic combinatorial optimization problem from linear algebra (the optimal Boolean solution x to $Ax=b$) via semidefinite program relaxation. A three-dimensional polyhedral analogue for the positive semidefinite cone of 3×3 symmetric matrices is introduced; a tool for visualizing in 6 dimensions. In "EDM proximity" we explore methods of solution to a few fundamental and prevalent Euclidean distance matrix proximity problems; the problem of finding that Euclidean distance matrix closest to a given matrix in the Euclidean sense. We pay particular attention to the problem when compounded with rank minimization. We offer a new geometrical proof of a famous result discovered by Eckart & Young in 1936 regarding Euclidean projection of a point on a subset of the positive semidefinite cone comprising all positive semidefinite matrices having rank not exceeding a prescribed limit ρ . We explain how this problem is transformed to a convex optimization for any rank ρ .

The Practice of Medicinal Chemistry - Camille Georges Wermuth 2003-06-11

The Practice of Medicinal Chemistry, 2E, is a single-volume source on the practical aspects of medicinal chemistry. The successful first edition was nicknamed "The Bible" by medicinal chemists, and the second edition has been updated, expanded and refocused to reflect developments over the last decade. Emphasis is put on how medicinal chemists conduct their search for and design of new drug entities. In contrast to competing books, it focuses on the chemistry rather than pharmacological concepts or descriptions of the various therapeutic classes of drugs. Most medicinal chemists working in the pharmaceutical industry are organic synthetic chemists who must acquire a strong knowledge of medicinal chemistry as they enter the industry. This book aims to be their practical handbook - a complete guide to the drug discovery process. * The only book available dealing with the practical aspects of medicinal chemistry * Serves as a complete guide to the drug discovery process, from conception of the molecules to drug production * Updated chapters devoted to the discovery of new lead compounds, including combinatorial chemistry

Bioinformatics and Biomedical Engineering - Ignacio Rojas 2019-04-30

The two-volume set LNBI 11465 and LNBI 11466 constitutes the proceedings of the 7th International Work-Conference on Bioinformatics and Biomedical Engineering, IWBBIO 2019, held in Granada, Spain, in May 2019. The total of 97 papers presented in the proceedings, was carefully reviewed and selected from 301 submissions. The papers are organized in topical sections as follows: Part I: High-throughput genomics: bioinformatics tools and medical applications; omics data acquisition, processing, and analysis; bioinformatics approaches for analyzing cancer sequencing data; next generation sequencing and sequence analysis; structural bioinformatics and function; telemedicine for smart homes and remote monitoring; clustering and analysis of biological sequences with optimization algorithms; and computational approaches for drug repurposing and personalized medicine. Part II: Bioinformatics for healthcare and diseases; computational

genomics/proteomics; computational systems for modelling biological processes; biomedical engineering; biomedical image analysis; and biomedicine and e-health.

Global Optimization - Marco Locatelli 2013-10-16

This volume contains a thorough overview of the rapidly growing field of global optimization, with chapters on key topics such as complexity, heuristic methods, derivation of lower bounds for minimization problems, and branch-and-bound methods and convergence. The final chapter offers both benchmark test problems and applications of global optimization, such as finding the conformation of a molecule or planning an optimal trajectory for interplanetary space travel. An appendix provides fundamental information on convex and concave functions. Intended for Ph.D. students, researchers, and practitioners looking for advanced solution methods to difficult optimization problems. It can be used as a supplementary text in an advanced graduate-level seminar. **Reviews in Computational Chemistry** - Kenny B. Lipkowitz 2009-09-22 Volume 11 **Reviews in Computational Chemistry** Kenny B. Lipkowitz and Donald B. Boyd The Theme of this Eleventh Volume is Computer-Aided Ligand Design and Modeling of Biomolecules. A Stellar Group of Scientists from Around the World Join in this Volume to Provide Tutorials for Beginners and Experts. Chapters 1 and 2 Take A Detailed Look at De Novo Design Methodologies for Discovering New Ligands which May Become Pharmaceuticals. Chapters 3 and 4 Cover the Methods and Applications of Three-Dimensional Quantitative Structure-Activity Relationships (3D-QSAR) Currently Used in Drug Discovery. Ways to Compute the Correct Lipophilic/Hydrophilic Behavior of Molecules are Taught in Chapter 5. Chapter 6 is an Exposition of Realistically Simulating DNA in the Complex Milieu of Ions that Surround it. An Appendix to this Volume Gives A Compendium of Software and Internet Tools for Computational Chemistry. -From Reviews of the Series . This Well-Respected Series Continues the Fine Selection of Topics and Presentation Qualities Set Forth by the Previous Members. For Example, Each Chapter Contains Thorough Treatment of the Theory Behind the Topic Being Covered. Moreover, the Background Material is Followed by Ample Timely Examples Culled From Recent Literature. *Journal of Medicinal Chemistry*

Global Optimization - Marco Locatelli 2013-10-16

This volume contains a thorough overview of the rapidly growing field of global optimization, with chapters on key topics such as complexity, heuristic methods, derivation of lower bounds for minimization problems, and branch-and-bound methods and convergence. The final chapter offers both benchmark test problems and applications of global optimization, such as finding the conformation of a molecule or planning an optimal trajectory for interplanetary space travel. An appendix provides fundamental information on convex and concave functions. Intended for Ph.D. students, researchers, and practitioners looking for advanced solution methods to difficult optimization problems. It can be used as a supplementary text in an advanced graduate-level seminar.

Recent Advances in Computational Optimization - Stefka Fidanova 2017-06-25

This book presents new optimization approaches and methods and their application in real-world and industrial problems, and demonstrates how many of the problems arising in engineering, economics and other domains can be formulated as optimization problems. Constituting a comprehensive collection of extended contributions from the 9th International Workshop on Computational Optimization (WCO) held in Gdansk, Poland, September 11-14, 2016, the book discusses important applications such as job scheduling, wildfire modeling, parameter settings for controlling different processes, capital budgeting, data mining, finding the location of sensors in a given network, identifying the conformation of molecules, algorithm correctness, decision support system, and computer memory management. Further, it shows how to develop algorithms for these based on new intelligent methods like evolutionary computations, ant colony optimization and constraint programming. The book is a valuable resource for researchers and practitioners alike.

Distance Geometry - Antonio Mucherino 2015-01-28

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.

Hemispherical Photography in Forest Science: Theory, Methods, Applications - Richard A. Fournier 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.

Encyclopedia of Bioinformatics and Computational Biology - 2018-08-21

Encyclopedia of Bioinformatics and Computational Biology: ABC of Bioinformatics combines elements of computer science, information technology, mathematics, statistics and biotechnology, providing the methodology and in silico solutions to mine biological data and processes. The book covers Theory, Topics and Applications, with a special focus on Integrative -omics and Systems Biology. The theoretical, methodological underpinnings of BCB, including phylogeny are covered, as are more current areas of focus, such as translational bioinformatics, cheminformatics, and environmental informatics. Finally, Applications provide guidance for commonly asked questions. This major reference work spans basic and cutting-edge methodologies authored by leaders in the field, providing an invaluable resource for students, scientists, professionals in research institutes, and a broad swath of researchers in biotechnology and the biomedical and pharmaceutical industries. Brings together information from computer science, information technology, mathematics, statistics and biotechnology Written and reviewed by leading experts in the field, providing a unique and authoritative resource Focuses on the main theoretical and methodological concepts before expanding on specific topics and applications Includes interactive images, multimedia tools and crosslinking to further resources and databases

Computational Topology in Image Context - Alexandra Bac 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.

Algebraic Geometry and Statistical Learning Theory - Sumio Watanabe 2009-08-13

Sure to be influential, Watanabe's book lays the foundations for the use of algebraic geometry in statistical learning theory. Many models/machines are singular: mixture models, neural networks, HMMs, Bayesian networks, stochastic context-free grammars are major examples. The theory achieved here underpins accurate estimation techniques in the presence of singularities.

Bioinformatics - Ralf Hofestädt 1997-08-06

This book constitutes the strictly refereed post-workshop proceedings of the German Conference on Bioinformatics, GCB'96, held in Leipzig, Germany, in September/October 1996. The volume presents 18 revised full papers together with three invited papers; these contributions were selected after a second round of reviewing from the 91 conference presentations. The book addresses current issues in computational biology and biologically inspired computing. The papers are organized in sections on biological and metabolic pathways, sequence analysis, molecular modeling, visualization, and formal languages, and DNA.

Euclidean Distance Geometry - Leo Liberti 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.

Topics in Semidefinite and Interior-Point Methods - Panos M. Pardalos and Henry Wolkowicz

This volume presents refereed papers presented at the workshop Semidefinite Programming and Interior-Point Approaches for Combinatorial Problems: held at The Fields Institute in May 1996. Semidefinite programming (SDP) is a generalization of linear programming (LP) in that the non-negativity constraints on the variables is replaced by a positive semidefinite constraint on matrix variables. Many of the elegant theoretical properties and powerful solution techniques follow through from LP to SDP. In particular, the primal-dual interior-point methods, which are currently so successful for LP, can be used to efficiently solve SDP problems. In addition to the theoretical and algorithmic questions, SDP has found many important applications in combinatorial optimization, control theory and other areas of mathematical programming. The papers in this volume cover a wide spectrum of recent developments in SDP. The volume would be suitable as a textbook for advanced courses in optimization. It is intended for graduate students and researchers in mathematics, computer science, engineering and operations.

Combinatorial Library Design and Evaluation - Arup Ghose 2001-06-26

This text traces developments in rational drug discovery and combinatorial library design with contributions from 50 leading scientists in academia and industry who offer coverage of basic principles, design strategies, methodologies, software tools and algorithms, and applications. It outlines the fundamentals of pharmacophore modelling and 3D Quantitative Structure-Activity Relationships (QSAR), classical QSAR, and target protein structure-based design methods.

Computer Algebra in Scientific Computing - François Boulier 2021-08-16

This book constitutes the proceedings of the 23rd International Workshop on Computer Algebra in Scientific Computing, CASC 2021, held in Sochi, Russia, in September 2021. The 24 full papers presented together with 1 invited talk were carefully reviewed and selected from 40 submissions. The papers cover theoretical computer algebra and its applications in scientific computing.

3D QSAR in Drug Design - Hugo Kubinyi 1993-12-31

Progress in medicinal chemistry and in drug design depends on our ability to understand the interactions of drugs with their biological targets. Classical QSAR studies describe biological activity in terms of physicochemical properties of substituents in certain positions of the drug molecules. The purpose of this book is twofold: On the one hand, both the novice and the experienced user will be introduced to the theory

and application of 3D QSAR analyses, and on the other, a comprehensive overview of the scope and limitations of these methods is given. The detailed discussion of the present state of the art should enable scientists to further develop and improve these powerful new tools. The greater part of the book is dedicated to the theoretical background of 3D QSAR and to a discussion of CoMFA applications. In addition, various other 3D QSAR approaches and some CoMFA-related methods are described in detail. Thus, the book should be valuable for medicinal, agricultural and theoretical chemists, biochemists and biologists, as well as for other scientists interested in drug design. Its content, starting at a very elementary level and proceeding to the latest methodological results, the strengths and limitations of 3D QSAR approaches, makes the book also appropriate as a text for teaching and for graduate student courses.

Mathematics of Bioinformatics - Matthew He 2011-03-16

Mathematics of Bioinformatics: Theory, Methods, and Applications provides a comprehensive format for connecting and integrating information derived from mathematical methods and applying it to the understanding of biological sequences, structures, and networks. Each chapter is divided into a number of sections based on the bioinformatics topics and related mathematical theory and methods. Each topic of the section is comprised of the following three parts: an introduction to the biological problems in bioinformatics; a presentation of relevant topics of mathematical theory and methods to the bioinformatics problems introduced in the first part; an integrative overview that draws the connections and interfaces between bioinformatics problems/issues and mathematical theory/methods/applications.

Geometric Science of Information - Frank Nielsen 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. *Handbook of Geometric Constraint Systems Principles* - Meera Sitharam 2018-07-20

The *Handbook of Geometric Constraint Systems Principles* is an entry point to the currently used principal mathematical and computational tools and techniques of the geometric constraint system (GCS). It functions as a single source containing the core principles and results, accessible to both beginners and experts. The handbook provides a guide for students learning basic concepts, as well as experts looking to pinpoint specific results or approaches in the broad landscape. As such, the editors created this handbook to serve as a useful tool for navigating the varied concepts, approaches and results found in GCS research. Key Features: A comprehensive reference handbook authored by top researchers Includes fundamentals and techniques from multiple perspectives that span several research communities Provides recent results and a graded program of open problems and conjectures Can be used for senior undergraduate or graduate topics course introduction to the area Detailed list of figures and tables About the Editors: Meera Sitharam is currently an Associate Professor at the University of Florida's Department of Computer & Information Science and Engineering. She received her Ph.D. at the University of Wisconsin, Madison. Audrey St. John is an Associate Professor of Computer Science at Mount Holyoke College, who received her Ph. D. from UMass Amherst. Jessica Sidman is a Professor of Mathematics on the John S. Kennedy Foundation at Mount Holyoke College. She received her Ph.D. from the University of Michigan.

The Methods of Distances in the Theory of Probability and Statistics - Svetlozar T. Rachev 2013-01-04

This book covers the method of metric distances and its application in probability theory and other fields. The method is fundamental in the study of limit theorems and generally in assessing the quality of approximations to a given probabilistic model. The method of metric distances is developed to study stability problems and reduces to the selection of an ideal or the most appropriate metric for the problem

under consideration and a comparison of probability metrics. After describing the basic structure of probability metrics and providing an analysis of the topologies in the space of probability measures generated by different types of probability metrics, the authors study stability problems by providing a characterization of the ideal metrics for a given problem and investigating the main relationships between different types of probability metrics. The presentation is provided in a general form, although specific cases are considered as they arise in the process of finding supplementary bounds or in applications to important special cases. Svetlozar T. Rachev is the Frey Family Foundation Chair of Quantitative Finance, Department of Applied Mathematics and Statistics, SUNY-Stony Brook and Chief Scientist of Finanalytica, USA. Lev B. Klebanov is a Professor in the Department of Probability and Mathematical Statistics, Charles University, Prague, Czech Republic. Stoyan V. Stoyanov is a Professor at EDHEC Business School and Head of Research, EDHEC-Risk Institute—Asia (Singapore). Frank J. Fabozzi is a Professor at EDHEC Business School. (USA)

Applications of Combinatorics and Graph Theory to the Biological and Social Sciences - Fred Roberts 2012-12-06

This IMA Volume in Mathematics and its Applications Applications of Combinatorics and Graph Theory to the Biological and Social Sciences is based on the proceedings of a workshop which was an integral part of the 1987-88 IMA program on APPLIED COMBINATORICS. We are grateful to the Scientific Committee: Victor Klee (Chairman), Daniel Kleitman, Dijen Ray-Chaudhuri and Dennis Stanton for planning and implementing an exciting and stimulating year long program. We especially thank the Workshop Organizers, Joel Cohen and Fred Roberts, for organizing a workshop which brought together many of the major figures in a variety of research fields connected with the application of combinatorial ideas to the social and biological sciences. A vner Friedman Willard Miller APPLICATIONS OF COMBINATORICS AND GRAPH THEORY TO THE BIOLOGICAL AND SOCIAL SCIENCES: SEVEN FUNDAMENTAL IDEAS FRED S. ROBERTS* Abstract. To set the stage for the other papers in this volume, seven fundamental concepts which arise in the applications of combinatorics and graph theory in the biological and social sciences are described. These ideas are: RNA chains as "words" in a 4 letter alphabet; interval graphs; competition graphs or niche overlap graphs; qualitative stability; balanced signed graphs; social welfare functions; and semiorders. For each idea, some basic results are presented, some recent results are given, and some open problems are mentioned.

Automata, Universality, Computation - Andrew Adamatzky 2014-11-15

This book is an intellectually stimulating excursion into mathematical machines and structures capable for a universal computation. World top experts in computer science and mathematics overview exciting and intriguing topics of logical theory of monoids, geometry of Gauss word, philosophy of mathematics in computer science, asynchronous and parallel P-systems, decidability in cellular automata, splicing systems, reversible Turing machines, information flows in two-way finite automata, prime generators in automaton arrays, Grossone and Turing machines, automaton models of atomic lattices. The book is full of visually attractive examples of mathematical machines, open problems and challenges for future research. Those interested in the advancement of a theory of computation, philosophy of mathematics, future and emergent computing paradigms, architectures and implementations will find the book vital for their research and development.

An Introduction to Distance Geometry applied to Molecular Geometry - Carlile Lavor 2017-07-12

This book is a pedagogical presentation aimed at advanced undergraduate students, beginning graduate students and professionals who are looking for an introductory text to the field of Distance Geometry, and some of its applications. This versions profits from feedback acquired at undergraduate/graduate courses in seminars and a number of workshops.

Bioinformatics and Biomedical Engineering - Francisco Ortuño 2015-04-01

The two volume set LNCS 9043 and 9044 constitutes the refereed proceedings of the Third International Conference on Bioinformatics and Biomedical Engineering, IWBBIO 2015, held in Granada, Spain in April 2015. The 134 papers presented were carefully reviewed and selected from 268 submissions. The scope of the conference spans the following areas: bioinformatics for healthcare and diseases, biomedical engineering, biomedical image analysis, biomedical signal analysis, computational genomics, computational proteomics, computational systems for modelling biological processes, eHealth, next generation

sequencing and sequence analysis, quantitative and systems pharmacology, Hidden Markov Model (HMM) for biological sequence modeling, advances in computational intelligence for bioinformatics and biomedicine, tools for next generation sequencing data analysis, dynamics networks in system medicine, interdisciplinary puzzles of measurements in biological systems, biological networks, high performance computing in bioinformatics, computational biology and computational chemistry, advances in drug discovery and ambient intelligence for bio emotional computing.

Measurement With Persons - Birgitta Berglund 2013-05-13

Measurements with persons are those in which human perception and interpretation are used for measuring complex, holistic quantities and qualities, which are perceived by the human brain and mind. Providing means for reproducible measurement of parameters such as pleasure and pain has important implications in evaluating all kind of products,

services, and conditions. This book inaugurates a new era for this subject: a multi- and inter-disciplinary volume in which world-renowned scientists from the psychological, physical, biological, and social sciences reach a common understanding of measurement theory and methods. In the first section, generic theoretical and methodological issues are treated, including the conceptual basis of measurement in the various fields involved; the development of formal, representational, and probabilistic theories; the approach to experimentation; and the theories, models, and methods for multidimensional problems. In the second section, several implementation areas are presented, including sound, visual, skin, and odor perception, functional brain imagining, body language and emotions, and, finally, the use of measurements in decision making. Measurement with Persons will appeal to a wide audience across a range of sciences, including general psychology and psychophysics, measurement theory, metrology and instrumentation, neurophysiology, engineering, biology, and chemistry.