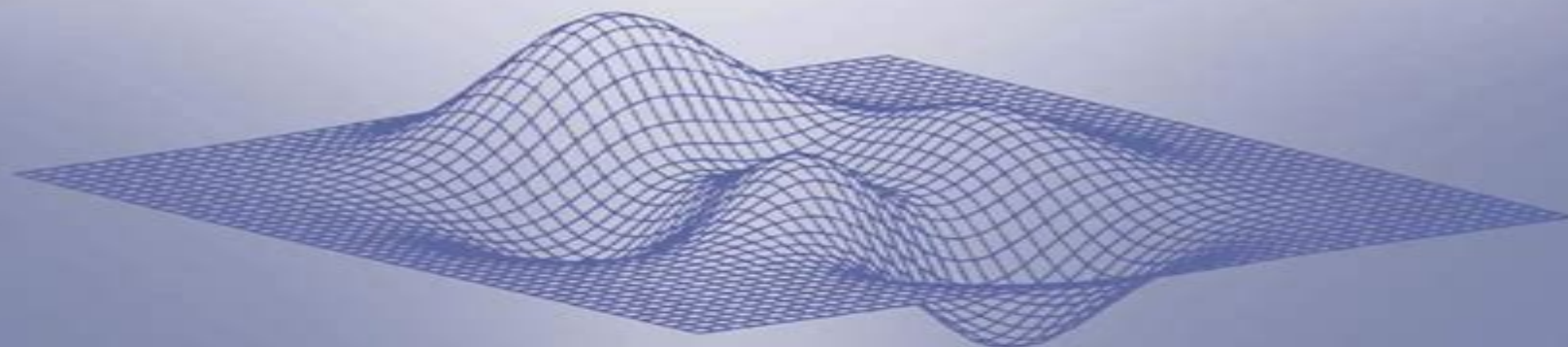


NONCONVEX OPTIMIZATION AND ITS APPLICATIONS

# **Optimization in Computational Chemistry and Molecular Biology**

**Local and Global Approaches**

C.A. Floudas and P.M. Pardalos (Eds.)



**Springer-Science+Business Media, B.V.**

# Optimization In Computational Chemistry And Molecular Biology Local And Global Approaches

**János D. Pintér**



## **Optimization In Computational Chemistry And Molecular Biology Local And Global Approaches:**

**Optimization in Computational Chemistry and Molecular Biology** Christodoulos A. Floudas, Panos M.

Pardalos, 2013-06-29 Optimization in Computational Chemistry and Molecular Biology Local and Global Approaches covers recent developments in optimization techniques for addressing several computational chemistry and biology problems A tantalizing problem that cuts across the fields of computational chemistry biology medicine engineering and applied mathematics is how proteins fold Global and local optimization provide a systematic framework of conformational searches for the prediction of three dimensional protein structures that represent the global minimum free energy as well as low energy biomolecular conformations Each contribution in the book is essentially expository in nature but of scholarly treatment The topics covered include advances in local and global optimization approaches for molecular dynamics and modeling distance geometry protein folding molecular structure refinement protein and drug design and molecular and peptide docking Audience The book is addressed not only to researchers in mathematical programming but to all scientists in various disciplines who use optimization methods in solving problems in computational chemistry and biology

**Optimization in Computational Chemistry and Molecular Biology** Christodoulos A. Floudas, Panos M.

Pardalos, 2000-02-29 Optimization in Computational Chemistry and Molecular Biology Local and Global Approaches covers recent developments in optimization techniques for addressing several computational chemistry and biology problems A tantalizing problem that cuts across the fields of computational chemistry biology medicine engineering and applied mathematics is how proteins fold Global and local optimization provide a systematic framework of conformational searches for the prediction of three dimensional protein structures that represent the global minimum free energy as well as low energy biomolecular conformations Each contribution in the book is essentially expository in nature but of scholarly treatment The topics covered include advances in local and global optimization approaches for molecular dynamics and modeling distance geometry protein folding molecular structure refinement protein and drug design and molecular and peptide docking Audience The book is addressed not only to researchers in mathematical programming but to all scientists in various disciplines who use optimization methods in solving problems in computational chemistry and biology

Optimization in Computational Chemistry and Molecular Biology Christodoulos A. Floudas, Panos Pardalos, 2014-01-15

**Lecture Notes on Computational Structural Biology** Zhijun Wu, 2008 While the field of computational structural biology or structural bioinformatics is rapidly developing there are few books with a relatively complete coverage of such diverse research subjects studied in the field as X ray crystallography computing NMR structure determination potential energy minimization dynamics simulation and knowledge based modeling This book helps fill the gap by providing such a survey on all the related subjects Comprising a collection of lecture notes for a computational structural biology course for the Program on Bioinformatics and Computational Biology at Iowa State University the book is in essence a comprehensive

summary of computational structural biology based on the author's own extensive research experience and a review of the subject from the perspective of a computer scientist or applied mathematician. Readers will gain a deeper appreciation of the biological importance and mathematical novelty of the research in the field. *Stochastic and Global Optimization* G. Dzemyda, V. Saltenis, A. Žilinskas, 2006-04-11. In the paper we propose a model of tax incentives optimization for investment projects with a help of the mechanism of accelerated depreciation. Unlike the tax holidays which influence on effective income tax rate, accelerated depreciation affects on taxable income. In modern economic practice the state actively use for an attraction of investment into the creation of new enterprises such mechanisms as accelerated depreciation and tax holidays. The problem under our consideration is the following. Assume that the state region is interested in realization of a certain investment project for example the creation of a new enterprise. In order to attract a potential investor the state decides to use a mechanism of accelerated tax depreciation. The following question arises: What is a reasonable principle for choosing depreciation rate? From the state's point of view the future investor's behavior will be rational. It means that while looking at economic environment the investor chooses such a moment for investment which maximizes his expected net present value NPV from the given project. For this case both criteria and investment rule depend on proposed by the state depreciation policy. For the simplicity we will suppose that the purpose of the state for a given project is a maximization of a discounted tax payments into the budget from the enterprise after its creation. Of course these payments depend on the moment of investor's entry and therefore on the depreciation policy established by the state. *Frontiers in Global Optimization* Christodoulos A. Floudas, Panos M. Pardalos, 2013-12-01. Global Optimization has emerged as one of the most exciting new areas of mathematical programming. Global optimization has received a wide attraction from many fields in the past few years due to the success of new algorithms for addressing previously intractable problems from diverse areas such as computational chemistry and biology, biomedicine, structural optimization, computer sciences, operations research, economics and engineering design and control. This book contains refereed invited papers submitted at the 4th international conference on Frontiers in Global Optimization held at Santorini, Greece during June 8-12, 2003. Santorini is one of the few sites of Greece with wild beauty created by the explosion of a volcano which is in the middle of the gulf of the island. The mystic landscape with its numerous mult extrema was an inspiring location particularly for researchers working on global optimization. The three previous conferences on Recent Advances in Global Optimization, State of the Art in Global Optimization and Optimization in Computational Chemistry and Molecular Biology Local and Global approaches took place at Princeton University in 1991, 1995 and 1999 respectively. The papers in this volume focus on deterministic methods for global optimization, stochastic methods for global optimization, distributed computing methods in global optimization and applications of global optimization in several branches of applied science and engineering: computer science, computational chemistry, structural biology and bioinformatics. **26th European Symposium on Computer Aided Process**

**Engineering** ,2016-06-17 26th European Symposium on Computer Aided Process Engineering contains the papers presented at the 26th European Society of Computer Aided Process Engineering ESCAPE Event held at Portoro Slovenia from June 12th to June 15th 2016 Themes discussed at the conference include Process product Synthesis Design and Integration Modelling Numerical analysis Simulation and Optimization Process Operations and Control and Education in CAPE PSE Presents findings and discussions from the 26th European Society of Computer Aided Process Engineering ESCAPE Event

Applications of Evolutionary Computation Giovanni Squillero,Paolo Burelli,2016-03-24 The two volumes LNCS 9597 and 9598 constitute the refereed conference proceedings of the 19th European Conference on the Applications of Evolutionary Computation EvoApplications 2016 held in Porto Portugal in March April 2016 co located with the Evo 2016 events EuroGP EvoCOP and EvoMUSART The 57 revised full papers presented together with 17 poster papers were carefully reviewed and selected from 115 submissions EvoApplications 2016 consisted of the following 13 tracks EvoBAFIN natural computing methods in business analytics and finance EvoBIO evolutionary computation machine learning and data mining in computational biology EvoCOMNET nature inspired techniques for telecommunication networks and other parallel and distributed systems EvoCOMPLEX evolutionary algorithms and complex systems EvoENERGY evolutionary computation in energy applications EvoGAMES bio inspired algorithms in games EvoIASP evolutionary computation in image analysis signal processing and pattern recognition EvoINDUSTRY nature inspired techniques in industrial settings EvoNUM bio inspired algorithms for continuous parameter optimization EvoPAR parallel implementation of evolutionary algorithms EvoRISK computational intelligence for risk management security and defence applications EvoROBOT evolutionary robotics and EvoSTOC evolutionary algorithms in stochastic and dynamic environments Handbook of Global Optimization Reiner

Horst,Panos M. Pardalos,H. Edwin Romeijn,2002-06-30 Global optimization is concerned with the computation and characterization of global optima of nonlinear functions During the past three decades the field of global optimization has been growing at a rapid pace and the number of publications on all aspects of global optimization has been increasing steadily Many applications as well as new theoretical algorithmic and computational contributions have resulted The Handbook of Global Optimization is the first comprehensive book to cover recent developments in global optimization Each contribution in the Handbook is essentially expository in nature but scholarly in its treatment The chapters cover optimality conditions complexity results concave minimization DC programming general quadratic programming nonlinear complementarity minimax problems multiplicative programming Lipschitz optimization fractional programming network problems trajectory methods homotopy methods interval methods and stochastic approaches **Introduction to Global**

**Optimization** R. Horst,Panos M. Pardalos,Nguyen Van Thoai,2000-12-31 Most of the existing books on optimization focus on the problem of computing locally optimal solutions Global optimization is concerned with the computation and characterization of global optima of nonlinear functions Global optimization problems are widespread in the mathematical

modeling of real world systems for a very broad range of applications During the past three decades many new theoretical algorithmic and computational contributions have helped to solve globally multi extreme problems arising from important practical applications Introduction to Global Optimization is the first comprehensive textbook that covers the fundamentals in global optimization The second edition includes algorithms applications and complexity results for quadratic programming concave minimization DC and Lipschitz problems decomposition algorithms for nonconvex optimization and nonlinear network flow problems Each chapter contains illustrative examples and ends with carefully selected exercises which are designed to help the student to get a grasp of the material and enhance their knowledge of global optimization methods Audience This textbook is addressed not only to students of mathematical programming but to all scientists in various disciplines who need global optimization methods to model and solve problems

**Theory and Applications of Computational Chemistry** Clifford Dykstra, Gernot Frenking, Kwang Kim, Gustavo Scuseria, 2011-10-13 Computational chemistry is a means of applying theoretical ideas using computers and a set of techniques for investigating chemical problems within which common questions vary from molecular geometry to the physical properties of substances Theory and Applications of Computational Chemistry The First Forty Years is a collection of articles on the emergence of computational chemistry It shows the enormous breadth of theoretical and computational chemistry today and establishes how theory and computation have become increasingly linked as methodologies and technologies have advanced Written by the pioneers in the field the book presents historical perspectives and insights into the subject and addresses new and current methods as well as problems and applications in theoretical and computational chemistry Easy to read and packed with personal insights technical and classical information this book provides the perfect introduction for graduate students beginning research in this area It also provides very readable and useful reviews for theoretical chemists Written by well known leading experts Combines history personal accounts and theory to explain much of the field of theoretical and computational chemistry Is the perfect introduction to the field

**Protein Modelling** Andrew Gamble, 2014-11-13 In this volume a detailed description of cutting edge computational methods applied to protein modeling as well as specific applications are presented Chapters include the application of Car Parrinello techniques to enzyme mechanisms the outline and application of QM MM methods polarizable force fields recent methods of ligand docking molecular dynamics related to NMR spectroscopy computer optimization of absorption distribution metabolism and excretion extended by toxicity for drugs enzyme design and bioinformatics applied to protein structure prediction A keen emphasis is laid on the clear presentation of complex concepts since the book is primarily aimed at Ph D students who need an insight in up to date protein modeling The inclusion of descriptive color figures will allow the reader to get a pictorial representation of complicated structural issues

**Deterministic Global Optimization** Christodoulos A. Floudas, 2013-03-09 The vast majority of important applications in science engineering and applied science are characterized by the existence of multiple minima and maxima as well as first second and higher order saddle points The

area of Deterministic Global Optimization introduces theoretical algorithmic and computational advances that i address the computation and characterization of global minima and maxima ii determine valid lower and upper bounds on the global minima and maxima and iii address the enclosure of all solutions of nonlinear constrained systems of equations Global optimization applications are widespread in all disciplines and they range from atomistic or molecular level to process and product level representations The primary goal of this book is three fold first to introduce the reader to the basics of deterministic global optimization second to present important theoretical and algorithmic advances for several classes of mathematical problems that include biconvex and bilinear problems signomial problems general twice differentiable nonlinear problems mixed integer nonlinear problems and the enclosure of all solutions of nonlinear constrained systems of equations and third to tie the theory and methods together with a variety of important applications

*Applied Optimization with MATLAB Programming* P. Venkataraman, 2009-03-23 Technology Engineering Mechanical Provides all the tools needed to begin solving optimization problems using MATLAB The Second Edition of *Applied Optimization with MATLAB Programming* enables readers to harness all the features of MATLAB to solve optimization problems using a variety of linear and nonlinear design optimization techniques By breaking down complex mathematical concepts into simple ideas and offering plenty of easy to follow examples this text is an ideal introduction to the field Examples come from all engineering disciplines as well as science economics operations research and mathematics helping readers understand how to apply optimization techniques to solve actual problems This Second Edition has been thoroughly revised incorporating current optimization techniques as well as the improved MATLAB tools Two important new features of the text are Introduction to the scan and zoom method providing a simple effective technique that works for unconstrained constrained and global optimization problems New chapter Hybrid Mathematics An Application using examples to illustrate how optimization can develop analytical or explicit solutions to differential systems and data fitting problems Each chapter ends with a set of problems that give readers an opportunity to put their new skills into practice Almost all of the numerical techniques covered in the text are supported by MATLAB code which readers can download on the text's companion Web site [www.wiley.com/go/venkat2e](http://www.wiley.com/go/venkat2e) and use to begin solving problems on their own This text is recommended for upper level undergraduate and graduate students in all areas of engineering as well as other disciplines that use optimization techniques to solve design problems

**Advances in Convex Analysis and Global Optimization** Nicolas Hadjisavvas, Panos M. Pardalos, 2013-12-01 There has been much recent progress in global optimization algorithms for nonconvex continuous and discrete problems from both a theoretical and a practical perspective Convex analysis plays a fundamental role in the analysis and development of global optimization algorithms This is due essentially to the fact that virtually all nonconvex optimization problems can be described using differences of convex functions and differences of convex sets A conference on Convex Analysis and Global Optimization was held during June 5-9 2000 at Pythagorion Samos Greece The conference was honoring

the memory of C Caratheodory 1873 1950 and was endorsed by the Mathematical Programming Society MPS and by the Society for Industrial and Applied Mathematics SIAM Activity Group in Optimization The conference was sponsored by the European Union through the EPEAEK program the Department of Mathematics of the Aegean University and the Center for Applied Optimization of the University of Florida by the General Secretariat of Research and Technology of Greece by the Ministry of Education of Greece and several local Greek government agencies and companies This volume contains a selective collection of refereed papers based on invited and contributing talks presented at this conference The two themes of convexity and global optimization pervade this book The conference provided a forum for researchers working on different aspects of convexity and global optimization to present their recent discoveries and to interact with people working on complementary aspects of mathematical programming      *Computational Science - ICCS 2003. Part 4.* Peter Sloot, 2003-05-22 The four volume set LNCS 2657 LNCS 2658 LNCS 2659 and LNCS 2660 constitutes the refereed proceedings of the Third International Conference on Computational Science ICCS 2003 held concurrently in Melbourne Australia and in St Petersburg Russia in June 2003 The four volumes present more than 460 reviewed contributed and invited papers and span the whole range of computational science from foundational issues in computer science and algorithmic mathematics to advanced applications in virtually all application fields making use of computational techniques These proceedings give a unique account of recent results in the field      Global Optimization János D. Pintér, 2006-10-13 Optimization models based on a nonlinear systems description often possess multiple local optima The objective of global optimization GO is to find the best possible solution of multiextremal problems This volume illustrates the applicability of GO modeling techniques and solution strategies to real world problems The contributed chapters cover a broad range of applications from agroecosystem management assembly line design bioinformatics biophysics black box systems optimization cellular mobile network design chemical process optimization chemical product design composite structure design computational modeling of atomic and molecular structures controller design for induction motors electrical engineering design feeding strategies in animal husbandry the inverse position problem in kinematics laser design learning in neural nets mechanical engineering design numerical solution of equations radiotherapy planning robot design and satellite data analysis The solution strategies discussed encompass a range of practically viable methods including both theoretically rigorous and heuristic approaches      *Multivalued Analysis and Nonlinear Programming Problems with Perturbations* B. Luderer, L. Minchenko, T. Satsura, 2013-03-09 The book presents a treatment of topological and differential properties of multivalued mappings and marginal functions In addition applications to sensitivity analysis of nonlinear programming problems under perturbations are studied Properties of marginal functions associated with optimization problems are analyzed under quite general constraints defined by means of multivalued mappings A unified approach to directional differentiability of functions and multifunctions forms the base of the volume Nonlinear programming problems involving quasidifferentiable functions are



considered as well A significant part of the results are based on theories and concepts of two former Soviet Union researchers Demyanov and Rubinov and have never been published in English before It contains all the necessary information from multivalued analysis and does not require special knowledge but assumes basic knowledge of calculus at an undergraduate level      *Computational Science - ICCS 2003. Part 3.* Peter Sloot,2003-05-22 The four volume set LNCS 2657 LNCS 2658 LNCS 2659 and LNCS 2660 constitutes the refereed proceedings of the Third International Conference on Computational Science ICCS 2003 held concurrently in Melbourne Australia and in St Petersburg Russia in June 2003 The four volumes present more than 460 reviewed contributed and invited papers and span the whole range of computational science from foundational issues in computer science and algorithmic mathematics to advanced applications in virtually all application fields making use of computational techniques These proceedings give a unique account of recent results in the field      **Neural Networks in Optimization** Xiang-Sun Zhang,2000-10-31 The book consists of three parts The first part introduces concepts and algorithms in optimization theory which have been used in neural network research The second part covers main neural network models and their theoretical analysis The third part of the book introduces various neural network models for solving nonlinear programming problems and combinatorial optimization problems Audience Graduate students and researchers who are interested in the intersection of optimization theory and artificial neural networks The book is appropriate for graduate courses

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