2022 年科学与工程计算青年研讨会

会 议 日 程

腾讯会议：228 227 670　密码：204204

日期	时间	报告信息
12 月 7 日（周三）	08:50－09:00	开幕式及合影，主持人：刘歆
	09:00－10:30	主持人：刘歆
	09:00－09:30	胡耀华（深圳大学） Mix Sparse Optimization: Theory and Applications
	09:30－10:00	丁　超（中国科学院数学与系统科学研究院） Recent Progress on Algorithm Foundation of Augmented Lagrangian Method
	10:00－10:30	江如俊（复旦大学） Solving Stackelberg Prediction Game with Least Squares Loss via Spherically Constrained Least Squares Reformulation
	10:30－10:50	茶　歇
	10:50－12:20	主持人：戴小英
	10:50－11:20	薛文超（中国科学院数学与系统科学研究院） 一类不确定系统的扩张状态滤波算法
	11:20－11:50	刘九龙（中国科学院数学与系统科学研究院） Generative Models Based Statistical Priors for Compressive Sensing Reconstruction
	11:50－12:20	张力维（加拿大英属哥伦比亚大学） A Generalized Atomic Cluster Expansion(ACE) Framework and its Applications in Electronic Structure Calculations
	12:20－14:00	午　休

	14:00－15:30	主持人：王旭
	14:00－14:30	顾　然（南开大学） A Random Active Set Method for Strictly Convex Quadratic Problem with Simple Bounds
	14:30－15:00	李　肖（香港中文大学深圳分校） A Unified Convergence Theorem for Stochastic Optimization Methods
	15:00－15:30	肖纳川（新加坡国立大学） Dissolving Constraints for Riemannian Optimization
	15:30－15:50	茶　歇
	15:50－17:20	主持人：崔涛
	15:50－16:20	胡凯博（牛津大学） Tensor Product Finite Element BGG Complexes
	16:20－16:50	吴朔男（北京大学） Discontinuous Galerkin Methods for Magnetic Advection-diffusion Problems
	16:50－17:20	王　旭（中国科学院数学与系统科学研究院） Inverse Random Potential Scattering for Biharmonic Waves
12 月 8 日 （周四）	09:00－10:30	主持人：殷涛
	09:00－09:30	林俊杉（奥本大学） Scattering Resonances Through Subwavelength Holes: Theory, Computation and Applications
	09:30－10:00	彭志超（密歇根州立大学） EM-WaveHoltz: a Flexible Frequency-domain Maxwell Solver Built from Time-domian Solvers
	10:00－10:30	李　浩（德克萨斯大学奥斯汀分校） On the Accuracy and Monotonicity of Spectral Element Method on Structured Meshes
	10:30－10:40	闭幕式，主持人：崔涛

附：报告题目与摘要

12 月 7 日

09:00－09:30
报告人：胡耀华（深圳大学）
报告题目：Mix Sparse Optimization: Theory and Applications
报告摘要： Structured sparse optimization has been extensively applied in the modelling of many important problems in various disciplines. The mix sparse structure is inherited in a wide class of practical applications, namely, the sparse structure appears as the inter-group and intra-group manners simultaneously. In this talk, we will discuss the nonconvex regularization method for mix sparse optimization problem, as well as a first-order iterative algorithm, and present its consistency theory, asymptotic theory and convergence theory. Applications of mix sparse optimization method to gene regulatory networks and differential optical absorption spectroscopy will be presented.

09:30－10:00
报告人：丁　超（中国科学院数学与系统科学研究院）
报告题目：Recent progress on algorithm foundation of augmented Lagrangian method
报告摘要： Strong variational sufficiency is a newly proposed property, which turns out to be of great use in the convergence analysis of multiplier methods. However, what this property implies for non-polyhedral problems remains a puzzle. In this talk, we prove the equivalence between the strong variational sufficiency and the strong second order sufficient condition (SOSC) for nonlinear semidefinite programming (NLSDP), without requiring the uniqueness of multiplier or any other constraint qualifications. Based on this characterization, the local convergence property of the augmented Lagrangian method (ALM) for NLSDP can be established under strong SOSC in the absence of constraint qualifications. Moreover, under the strong SOSC, we can apply the semi-smooth Newton method to solve the ALM subproblems of NLSDP as the positive definiteness of the generalized Hessian of augmented Lagrangian function is satisfied.

10: 00－10:30

报告人：江如俊（复旦大学）

报告题目：Solving Stackelberg Prediction Game with Least Squares Loss via Spherically

报告摘要：The Stackelberg prediction game (SPG) is popular in characterizing strategic interactions between a learner and an attacker. As an important special case, the SPG with least squares loss (SPG-LS) has recently received much research attention. Although initially formulated as a difficult bi-level optimization problem, SPG-LS admits tractable reformulations which can be polynomially globally solved by semidefinite programming or second order cone programming. However, all the available approaches are not well-suited for handling large-scale datasets, especially those with huge numbers of features. In this paper, we explore an alternative reformulation of the SPG-LS. By a novel nonlinear change of variables, we rewrite the SPG-LS as a spherically constrained least squares (SCLS) problem. Theoretically, we show that an ϵ optimal solutions to the SCLS (and the SPG-LS) can be achieved in $\tilde O(N/\sqrt{\epsilon})$ floating-point operations, where N is the number of nonzero entries in the data matrix. Practically, we apply two well-known methods for solving this new reformulation, i.e., the Krylov subspace method and the Riemannian trust region method. Both algorithms are factorization free so that they are suitable for solving large scale problems. Numerical results on both synthetic and real-world datasets indicate that the SPG-LS, equipped with the SCLS reformulation, can be solved orders of magnitude faster than the state of the art.

10:50－11:20

报告人：薛文超（中国科学院数学与系统科学研究院）

报告题目：一类不确定系统的扩张状态滤波算法

报告摘要：本报告首先针对一类具有非线性不确定动态及扰动的系统，给出了系统可观的条件以及扩张状态卡尔曼滤波的设计方法。进一步在未知动态和随机性噪声同时存在下，证明了滤波算法的稳定性、一致性，以及在一定条件下的渐近最优性，并介绍了一些实际系统的应用。最后给出了传器网络下的分布式扩张状态卡尔曼滤波算法以及相应稳定性等结果。

11:20－11:50

报告人：刘九龙（中国科学院数学与系统科学研究院）

报告题目：Generative Models Based Statistical Priors for Compressive Sensing Reconstruction

报告摘要：Sparsity is a mathematically elegant tool for reducing the sampling rate for compressive sensing reconstruction and thereby its applications are also extended to many underdetermined imaging systems, such as MRI and CT. However, as the development of the deep learning, there are many methods are proposed to learn data representation and they are shown to be more efficient in signal and image processing. In order to efficiently and stably solve the under-determined and ill-conditioned inverse problems with fewer measurements, we established compressive sensing reconstruction methods using generative priors which are shown much more efficient than the traditional priors or some other data-driven priors. In this talk, I will introduce some of these methods and present our recent results for MRI reconstruction, phase retrieval, and some other nonlinear inverse problems.

11:50－12:20

报告人：张力维（加拿大英属哥伦比亚大学）

报告题目：A generalized Atomic Cluster Expansion(ACE) framework and its applications in electronic structure calculations

报告摘要：Atomic Cluster Expansion(ACE) [Drautz, 2019] gives rise to a powerful tool for approximating isometry invariant properties. There are also many other properties of interest that have different physical symmetries under some abstract group actions. In this talk, I will introduce a generalized ACE framework, which provides an error-controllable way to approximate symmetric properties for many body systems. In particular, one of its implementations in electronic structure calculations will be introduced in detail.

14:00－14:30

报告人：顾　然（南开大学）

报告题目：A Random Active Set Method For Strictly Convex Quadratic Problem With Simple Bounds

报告摘要： The active set method aims at finding the correct active set of the optimal solution and it is a powerful method for solving strictly convex quadratic problem with bound constraints. To guarantee the finite step convergence, the existing active set methods all need strict conditions or some additional strategies, which greatly affect the efficiency of the algorithm. In this talk, we propose a random active set method which introduces randomness in the update of active set. We prove that it can converge in finite number of iterations with probability one without extra conditions on the problem or any additional strategies. Numerical experiments show that the algorithm can obtain the correct active set within a few iterations, and it has better efficiency and robustness than the existing methods.

14:30－15:00

报告人：李　肖（香港中文大学深圳分校）

报告题目：A Unified Convergence Theorem for Stochastic Optimization Methods

报告摘要： In this talk, I will present a fundamental unified convergence theorem used for deriving expected and almost sure convergence results for a series of stochastic optimization methods. Our unified theorem only requires to verify several representative conditions and is not tailored to any specific algorithm. As a direct application, we recover expected and almost sure convergence results of the stochastic gradient method (SGD) and random reshuffling (RR) under more general settings. Moreover, we establish new expected and almost sure convergence results for the stochastic proximal gradient method (prox-SGD) and stochastic model-based methods (SMM) for nonsmooth nonconvex optimization problems. These applications reveal that our unified theorem provides a plugin-type convergence analysis and strong convergence guarantees for a wide class of stochastic optimization methods.

15:00－15:30

报告人：肖纳川（新加坡国立大学）

报告题目：Dissolving Constraints for Riemannian Optimization

报告摘要： This talk proposes a class of constraint dissolving approaches for optimization problems over closed Riemannian manifolds. In these proposed approaches, solving a Riemannian optimization problem is transferred into the unconstrained minimization of a constraint dissolving function named CDF. Different from existing exact penalty functions, the exact gradient and Hessian of CDF are easy to compute. We study the theoretical properties of CDF and prove that the original problem and CDF have the same first-order and second-order stationary points, local minimizers, and {\L}ojasiewicz exponents in a neighborhood of the feasible region. Remarkably, the convergence properties of our proposed constraint dissolving approaches can be directly inherited from the existing rich results in unconstrained optimization. Therefore, the proposed constraint dissolving approaches build up short cuts from unconstrained optimization to Riemannian optimization.

Moreover, we introduce CDOpt (available at \url{https://cdopt.github.io/} under BSD 3-clause license), a user-friendly Python package for a class of Riemannian optimization. Based on the constraint dissolving approaches, the Riemannian optimization problems are transformed into their equivalent unconstrained counterparts in CDOpt. Therefore, solving Riemannian optimization problems through CDOpt directly benefits from various existing solvers and the rich expertise gained over decades for unconstrained optimization. Extensive numerical experiments demonstrate the high efficiency and robustness of CDOpt in solving various classes of Riemannian optimization problems.

15:50－16:20

报告人：胡凯博（牛津大学）

报告题目：Tensor product finite element BGG complexes

报告摘要： We construct spline and finite element versions of Bernstein-Gelfand-Gelfand (BGG) sequences in any space dimension. Examples in 3D include the elasticity, the Hessian, and the div div complexes. The resulting spaces and complexes are tensor products of 1D complexes with various kinds of regularity. The tensor product structure also leads to bounded commuting quasi-interpolations.

16:20－16:50

报告人：吴朔男（北京大学）

报告题目： Discontinuous Galerkin methods for magnetic advection-diffusion problems

报告摘要： We devise and analyze a class of the primal discontinuous Galerkin methods for magnetic advection-diffusion problems based on the weighted-residual approach. In addition to the upwind stabilization, we find a new mechanism under the vector case that provides more flexibility in constructing the schemes. For the more general Friedrichs system, we show the stability and optimal error estimate, which boil down to two core ingredients -- the weight function and the special projection -- that contain information of advection. Numerical experiments are provided to verify the theoretical results.

16:50－17:20

报告人：王旭（中国科学院数学与系统科学研究院）

报告题目：Inverse random potential scattering for biharmonic waves

报告摘要：Scattering problems have been widely investigated for acoustic, elastic,and electromagnetic waves. Recently, scattering problems for biharmonic waves have attracted much attention due to significant applications in thin plate elasticity. This talk is concerned with an inverse random potential scattering problem for the biharmonic wave equation, where the potential is modeled as a microlocally isotropic Gaussian rough field. For the direct scattering problem, the well-posedness is established and the regularity of the solution is obtained by developing a new unique continuation theorem for the stochastic biharmonic wave equation. For the inverse scattering problem, the statistical strength of the random potential is shown to be uniquely determined by the high frequency limit of the second moment of the scattered field averaged over the frequency band. Moreover, we show that the expectation can be removed and only a single realization is required to ensure the uniqueness of the inverse problem when the medium is lossless.

12 月 8 日

09:00－09:30

报告人：林俊杉（奥本大学）

报告题目：Scattering Resonances Through Subwavelength Holes: Theory, Computation and Applications

报告摘要：The so-called extraordinary optical transmission (EOT) through metallic nanoholes has triggered extensive research in modern plasmonics and their applications in bio-sensing, imaging, etc. In this talk, I will give an overview of quantitative mathematical theory to understand a variety of resonances that induce the EOT phenomenon, the computational methods for solving the underlying multiscale problems, and the mathematical studies for their applications in imaging and sensing.

09:30－10:00

报告人：彭志超（密歇根州立大学）

报告题目：EM-WaveHoltz: a flexible frequency-domain Maxwell solver built from time-domian solvers

报告摘要：Two challenges to design efficient iterative solvers for the frequency-domain Maxwell equations are the indefinite nature of the underlying system and the high resolution requirements. Scalable parallel frequency-domain Maxwell solvers are highly desired.

This talk will introduce the EM-WaveHoltz method which builds frequency-domain Maxwell solvers from time-domain solvers. Three main advantages of the proposed method are as follows. (1) It results in a better conditioned linear system which is proved to be SPD in special cases. (2) It is flexible and simple to convert time-domain solvers to efficient frequency-domain solvers. (3) It is possible to obtain solutions for multiple frequencies in one solve. The formulation of the EM-WaveHoltz will be introduced, and its performance will be demonstrated through numerical experiments.

10: 00－10:30

报告人：李　浩（德克萨斯大学奥斯汀分校）

报告题目：On the Accuracy and Monotonicity of Spectral Element Method on Structured Meshes

报告摘要：In the literature, spectral element methods usually refer to finite element methods with high order polynomial basis. The Q^k spectral element method has been a popular high order method for solving second order PDEs, e.g., wave equations, obtained by continuous finite element method with tenor product polynomial of degree k and with at least (k+1)-point Gauss-Lobatto quadrature. I will present some new results of this classical scheme, include its accuracy, monotonicity (stability) and a finite difference implementation of Q^2 spectral element method which is monotone for the variable coefficient Poisson equation therefore satisfies the discrete maximum principle. Such a scheme can be proven to be fourth order accurate. This is the first time that a high order accurate scheme that is proven to satisfy the discrete maximum principle for a variable coefficient diffusion operator.