### 第八届北京大学计算与应用数学拔尖博士生研讨会 暨第十一届北京计算数学研究生论坛

为促进计算与应用数学领域优秀博士生之间的互学互鉴,搭建展示成果、交流学习、了解前沿、自由讨论的学术平台,第八届北京大学计算与应用数学 拔尖博士生研讨会暨第十一届北京计算数学研究生论坛将于 2025 年 11 月 17 日 -11 月 19 日在北京大学举行。期待与会者通过此次研讨,提升学术表达能力,拓宽研究视野,增强创新意识,激发科研热情,坚定攻坚克难的决心与信心,实现共同进步。

#### 会议时间

2025年11月17日14:00至17:00 2025年11月18日09:00至17:00 2025年11月19日09:00至16:00

#### 会议地点

北京大学智华楼 101 王选报告厅

#### 主办单位

国家自然科学基金委员会基础科学中心 北京大学数学科学学院 北京国际数学研究中心 北京大学国际机器学习研究中心

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张振毅 北京大学

会议日程						
时间	11月17日	11月18日	11月19日			
09:00-10:00		<b>邀请报告</b> 胡天昊 戴咏诚	<b>邀请报告</b> 杨 俨 侯 頔			
10:00-10:30		茶 歇				
10:30-12:00		<b>邀请报告</b> 吴佩颖 林 野 李柄辉	<b>邀请报告</b> 单佳骊 邓一理 金振远			
12:00-14:00	报 到	午 休				
14:00-15:00	<b>开幕式</b> <b>大会报告</b> 胡凯博	<b>邀请报告</b> 陈玉祥 段嘉怡	<b>邀请报告</b> 谢宝玲 刘帅军			
15:00-15:30	茶	歇	李英恺			
15:30-17:00	<b>邀请报告</b> 汪锴波 吴亚昊 张振毅	<b>邀请报告</b> 张梦晴 蔡泽宇				
17:00-19:00		晚宴				

11月17日					
时 间	报告人	题目	主持人		
14:00-14:15	开幕式与合影				
14:15-15:00	大会报告 胡凯博 <sub>牛津大学</sub>	Towards computational topological hydrodynamics: relaxation, dynamo, finite element exterior calculus			
15:00-15:30	茶歇				
15:30-16:00	<b>张振毅</b> 北京大学	Towards a Mathematical View of AI Virtual Cells: When Generative Modeling Meets Optimal Transport			
16:00-16:30	<b>汪锴波</b> 香港科技大学	Towards a Golden Classifier-Free Guidance Path via Foresight Fixed Point Iterations	刘宇扬		
16:30-17:00	<b>吴亚昊</b> 西安交通大学	耦合潜变量生成模型的变分推断 方法及其应用			

11月18日					
时间	报告人	题目	主持人		
09:00-09:30	<b>胡天昊</b> 香港中文大学	An Iterative Deep Ritz Method for Monotone Elliptic Problems	ms 一 李晨毅 rol		
09:30-10:00	<b>戴咏诚</b> 南方科技大学	Solving Elliptic Optimal Control Problems via Neural Networks and Optimality System			
10:00-10:30		茶歇			
10:30-11:00	<b>吴佩颖</b> 武汉大学	DRM Revisited: A Complete Error Analysis	苏 华		
11:00-11:30	<b>林 野</b> 吉林大学	基于神经网络的格林函数估计 与算子学习方法研究			
11:30-12:00	<b>李柄辉</b> 北京大学	Functional Scaling Laws in Kernel Regression: Loss Dynamics and Learning Rate Schedules			
12:00-14:00	午休				
14:00-14:30	<b>蔡泽宇</b> 中国科学技术大学				
14:30-15:00	<b>张梦晴</b> 北京应用物理 与计算数学研究所	时空一致高效高精度的 DG-HGKS 算法研究	郭宇扬		
15:00-15:30		茶歇			
15:30-16:00	<b>段嘉怡</b> 香港理工大学	A third-order structure-preserving exponential time differencing Runge-Kutta scheme for the binary fluid-surfactant phase field model	- 武朔南		
16:00-16:30	<b>陈玉祥</b> 厦门大学	Energy stable finite element approximations of gas flow in poroelastic media			
17:00-19:00		<b>晚宴</b> 勺园中餐厅朗润厅			

11月19日				
时 间	报告人	题目	主持人	
09:00-09:30	杨 俨 中国科学院 数学与系统科学研究院	A space-decoupling framework for optimization on bounded-rank matrices with orthogonally invariant constraints	王修远	
09:30-10:00	<b>侯 頔</b> 新加坡国立大学	RiNNAL+: a Riemannian ALM Solver for SDP-RLT Relaxations of Mixed-Binary Quadratic Programs	of	
10:00-10:30		茶歇		
10:30-11:00	<b>单佳骊</b> <sub>复旦大学</sub>	i least sollares and its		
11:00-11:30	<b>邓一理</b> 清华大学	, —   · · · · · · · · · · · · · · · · · ·		
11:30-12:00	<b>金振远</b> 上海交通大学	Interference-Free Propagation: Achieving Reliable Signal Propagation in Brain Networks with Areal-Specific Local Dynamics		
12:00-14:00	午休			
14:00-14:30	<b>谢宝玲</b> <sub>浙江大学</sub>	A singularity guided Nyström method for 2D elastostatics with corners		
14:30-15:00	<b>刘帅军</b> 四川大学	1 17 1		
15:00-15:30	<b>李英恺</b> 北京师范大学	Error estimates of the Strang splitting scaled LaguerreFourier pseudospectral method for the GrossPitaevskii equation with angular momentum rotation		

# Towards computational topological hydrodynamics: relaxation, dynamo, finite element exterior calculus

#### 胡凯博

#### 牛津大学

Fluid mechanics and magnetohydrodynamics often involve intricate differential and topological structures, such as vorticity and magnetic field knots, which are critical to the underlying physics. Numerical discretization errors can break these structures, leading to wrong solutions.

In this talk, we present two examples in topological (magneto)hydrodynamics: relaxation and dynamo. Relaxation addresses the evolution of magnetic fields from given initial conditions in plasma physics, focusing on the existence and properties of stationary states. Open questions, including the Parker hypothesis, highlight the role of magnetic field line topology, particularly knots, in constraining relaxation processes. Conversely, the dynamo problem examines the exponential growth of magnetic fields.

We emphasize the importance of structure-preserving numerical methods, specifically those that conserve helicity and topology. Using finite element de Rham complexes within the framework of finite element exterior calculus, we derive schemes that precisely preserve these structures, ensuring robust and physically meaningful simulations.

Short Bio: Kaibo Hu is a Senior Research Fellow and Associate Professor at the Mathematical Institute, University of Oxford, and a Royal Society University Research Fellow. His research focuses on numerical partial differential equations and structure-preserving discretizations, particularly on finite element exterior calculus (FEEC) and applications.

Kaibo Hu earned a PhD from Peking University in 2017, followed by postdoctoral positions at the University of Oslo and the University of Minnesota, and a Hooke Research Fellowship at University of Oxford. After serving as a Reader at the University of Edinburgh, he joined Oxford in 2025. He received the SIAM Computational Science and Engineering Early Career Prize (2023), and is the PI of the ERC Starting Grant project GeoFEM (Geometric Finite Element Methods).

# Towards a Mathematical View of AI Virtual Cells: When Generative Modeling Meets Optimal Transport

#### 张振毅

#### 北京大学

Reconstructing continuous cellular dynamics from sparse, high-dimensional single-cell omics data remains a fundamental challenge in computational biology. Recently, a paradigm shift has been witnessed by leveraging artificial intelligence—specifically, dynamical generative modeling—to develop an AI virtual cell, a predictive digital twin capable of simulating cellular behavior across time and space. In this talk, we introduce our recent attempts that integrate generative AI models with partial differential equations (PDEs) and optimal transport (OT) theory to infer latent dynamics from scRNA-seq data. To further infer stochastic dynamics from static data, we explore a regularized unbalanced optimal transport (RUOT) formulation and its theoretical connections to the Schrödinger Bridge and diffusion models. We also consider extending this theory to spatial transcriptomics data and incorporating cell-cell communications. Together, these works suggest how generative AI and mathematical tools could work together to unify dynamical modeling, spatial reconstruction, and stochastic inference, transforming fragmented omics data into a predictive virtual cell.

个人简介: 张振毅, 北京大学数学科学学院, 研究方向为生成建模, 数据驱动的动力学与计算方法, 在 ICLR, NeurIPS, Advanced Science, Communications in Computational Physics等学术会议或期刊发表论文, 相关工作获得 ICLR 大会口头报告。

# Towards a Golden Classifier-Free Guidance Path via Foresight Fixed Point Iterations

#### 汪锴波

#### 香港科技大学

Classifier-Free Guidance (CFG) is an essential component of text-to-image diffusion models, and understanding and advancing its operational mechanisms remains a central focus of research. Existing approaches stem from divergent theoretical interpretations, thereby limiting the design space and obscuring key design choices. To address this, we propose a unified perspective that reframes conditional guidance as fixed point iterations, seeking to identify a golden path where latents produce consistent outputs under both conditional and unconditional generation. We demonstrate that CFG and its variants constitute a special case of single-step short-interval iteration, which is theoretically proven to exhibit inefficiency. To this end, we introduce Foresight Guidance (FSG), which prioritizes solving longer-interval subproblems in early diffusion stages with increased iterations. Extensive experiments across diverse datasets and model architectures validate the superiority of FSG over state-of-the-art methods in both image quality and computational efficiency. Our work offers novel perspectives for conditional guidance and unlocks the potential of adaptive design.

个人简介: 汪锴波, 2020 年于浙江大学获自动化学士学位, 2023 年于浙江 大学获控制理论与控制工程硕士学位, 2023 年至今于香港科技大学概率与统计 方向攻读博士学位, 导师为项阳教授。主要研究方向为对抗攻击与防御、扩散 模型等。

#### 耦合潜变量生成模型的变分推断方法及其应用

#### 吴亚昊

#### 西安交通大学

随着单细胞转录组技术的发展,构建扰动条件下的细胞响应模型已成为生物统计领域的重要研究问题。然而,受实验成本与可观测性限制,真实扰动数据往往难以充分获取。为此,本文提出一种基于变分推断的概率生成模型——CoupleVAE,用于对受控与扰动条件下的单细胞表达分布进行联合建模、推断与预测。我们构建了一个由耦合潜变量组成的概率图模型,其中两组潜变量分别对应扰动前与扰动后条件下的潜在细胞状态,并通过可学习的非线性潜空间映射刻画扰动诱导的跨条件分布变换。在推断过程中,模型通过最小化潜在后验与先验分布之间的 KL 散度,最大化联合似然的变分证据下界(ELBO),从而实现对跨条件潜变量的变分贝叶斯近似推断。在 COVID-19 感染、IFN-B 刺激及跨物种 LPS 数据上的对比实验表明,CoupleVAE 在分布拟合精度、差异基因识别能力及跨分布泛化性方面均优于现有深度生成模型。该方法为单细胞扰动响应建模、因果于预预测及跨条件表达生成提供了一种新的统计推断范式。

个人简介:吴亚昊,2021 年本科毕业于西安交通大学数学与应用数学专业,现为西安交通大学统计学专业博士研究生。主要研究方向为生物统计学与深度学习方法在单细胞数据分析中的应用。

#### An Iterative Deep Ritz Method for Monotone Elliptic Problems

#### 胡天昊

#### 香港中文大学

In this work, we present a novel iterative deep Ritz method (IDRM) for solving a general class of elliptic problems. It is inspired by the iterative procedure for minimizing the loss during the training of the neural network, but at each step encodes the geometry of the underlying function space and incorporates a convex penalty to enhance the performance of the algorithm. The algorithm is applicable to elliptic problems involving a monotone operator (not necessarily of variational form) and does not impose any stringent regularity assumption on the solution. It improves several existing neural PDE solvers, e.g., physics informed neural network and deep Ritz method, in terms of the accuracy for the concerned class of elliptic problems. Further, we establish a convergence rate for the method using tools from geometry of Banach spaces and theory of monotone operators, and also analyze the learning error. To illustrate the effectiveness of the method, we present several challenging examples, including a comparative study with existing techniques.

个人简介: 胡天昊,本科毕业于吉林大学唐敖庆理科试验班,现于香港中文大学数学系攻读博士学位。本科期间曾获国家奖学金,并荣获校十佳大学生、优秀毕业生等称号。目前主要研究方向包括偏微分方程数值解、科学计算及反问题计算方法,已在 SIAM Journal on Scientific Computing、Journal of Computational Physics 等计算数学领域高水平期刊上发表多篇论文。此外,他还 受 邀 在 多 个 知 名 学 术 会 议 上 作 报 告 ,包 括 SIAM Conference on Computational Science and Engineering 以及第十四届反问题成像及应用会议等。

### Solving Elliptic Optimal Control Problems via Neural Networks and Optimality System

#### 戴咏诚

#### 南方科技大学

In this work, we investigate a neural network based solver for optimal control problems (without/with box constraint) for linear and semilinear second-order elliptic problems. It utilizes a coupled system derived from the first-order optimality system of the optimal control problem, and employs deep neural networks to represent the solutions to the reduced system. We present an error analysis of the scheme, and provide  $L^2(\Omega)$  error bounds on the state, control and adjoint in terms of neural network parameters (e.g., depth, width, and parameter bounds) and the numbers of sampling points. The main tools in the analysis include offset Rademacher complexity and boundedness and Lipschitz continuity of neural network functions. We present several numerical examples to illustrate the method and compare it with two existing ones.

个人简介: 戴咏诚, 2022 毕业于浙江大学信息与计算科学专业, 现为南方科技大学与香港理工大学联合培养博士, 主要研究兴趣为: 微分方程数值解, 反问题, 机器学习, 非局部模型。

#### **DRM Revisited: A Complete Error Analysis**

#### 吴佩颖

#### 武汉大学

本文在过参数化设置下,首次为 Deep Ritz 方法 (DRM) 提供了同时涵盖逼近误差、泛化误差和优化误差的完整误差分析。具体来说,利用深度学习方法求解偏微分方程 (PDE) 时,完整的误差分析通常需包含逼近、泛化和优化三部分误差。现有理论工作多在神经网络欠参数化设置下权衡逼近与泛化误差,或在过参数化设置下单独分析优化误差。但遗憾的是,这两种分析范式难以融合,如何统一分析三类误差仍面临重大挑战。为填补这一理论空白,本文以求解二阶椭圆型方程的 Deep Ritz 方法为对象,首次在过参数化框架下,建立了一套同时包含逼近、泛化和优化误差的完整分析框架。该框架允许网络参数在训练过程中显著偏离初始值,并从理论上回答了深度 PDE 求解领域的一个关键问题:给定目标精度,应如何协同配置网络结构、样本数量、学习率与迭代次数等关键超参数,以确保算法输出达到预期精度。

个人简介: 吴佩颖, 武汉大学数学与统计学院博士生, 研究方向为深度神经网络求解 pde 的误差分析以及机器学习理论。

#### 基于神经网络的格林函数估计与算子学习方法研究

#### 林野

#### 吉林大学

近年来,人工智能与科学计算的深度融合已成为前沿研究热点,其中,偏 微分方程(PDE)的数值求解是关键问题之一。算子学习方法可有效泛化求解 PDE,深度格林网络(GL)方法通过神经网络逼近 PDE 的格林函数,将算子学 习问题转化为核函数估计问题, 兼具物理可解释性与数据驱动的优势。但核函 数估计中存在的三个主要问题: 奇异性难以逼近、积分计算复杂度高以及深度 网络训练不稳定。首先,我们提出了 GreenMGNet,一种基于深度神经网络的高 性能核函数估计方法。该方法通过超平面划分定义域来处理格林函数的奇异性, 并设计了增广神经网络(AugNN)来捕捉不光滑特征。同时,结合多级多积分算 法(MLMI)将积分计算复杂度降至近线性,显著提升了在训练与推理阶段的整 体计算效率与精度。其次,针对深度网络的训练难题,我们提出了基于浅层神 经网络的高精度核函数估计方法。通过定义基于积分的新半内积,我们设计了 正交贪婪算法(OGA)并在理论上证明了其逼近速率。为进一步突破维数障碍, 我们提出了逐点正交贪婪算法(PW-OGA),将高维问题分解为多个低维问题进行 求解。实验表明,该方法将逼近误差较深度网络基线降低了数个数量级。数值 实验证明, GreenMGNet 在计算效率上显著优于传统 GL 方法, 而 OGA 与 PW-OGA 则在逼近精度上展现了巨大优势,分别从"高效率"和"高精度"两个维度推 进了基于神经网络的核函数估计方法,为科学计算提供了更可靠、更高效的 PDE 求解工具。

个人简介: 林野, 吉林大学计算数学 2021 级博士生。

# **Functional Scaling Laws in Kernel Regression: Loss Dynamics and Learning Rate Schedules**

#### 李柄辉

#### 北京大学

Scaling laws have emerged as a unifying lens for understanding and guiding the training of large language models (LLMs). However, existing studies predominantly focus on the final-step loss, leaving open whether the entire loss dynamics obey similar laws and, crucially, how the learning rate schedule (LRS) shapes them. We address these gaps in a controlled theoretical setting by analyzing stochastic gradient descent (SGD) on a power-law kernel regression model. The key insight is a novel intrinsictime viewpoint, which captures the training progress more faithfully than iteration count. We then establish a Functional Scaling Law (FSL) that captures the full loss trajectory under arbitrary LRSs, with the schedule's influence entering through a simple convolutional functional. We further instantiate the theory for three representative LRSs---constant, exponential decay, and warmup-stable-decay (WSD)---and derive explicit scaling relations in both data- and compute-limited regimes. These comparisons explain key empirical phenomena: (i) higher-capacity models are more data- and compute-efficient; (ii) learning-rate decay improves training efficiency; and (iii) WSDtype schedules outperform pure decay. Finally, experiments on LLMs ranging from 0.1B to 1B parameters demonstrate the practical relevance of FSL as a surrogate model for fitting and predicting loss trajectories in large-scale pre-training.

个人简介:李柄辉,北京大学国际机器学习研究中心 2023 级博士生,研究方向为深度学习理论。

### Discontinuous Galerkin solutions of all-electron Kohn-Sham equation

#### 蔡泽宇

#### 中国科学技术大学

With the growing interest in simulating phenomena such as Auger effects, allelectron density functional theory faces increasing computational challenges. In this talk, I will present a discontinuous Galerkin framework for solving the all-electron Kohn–Sham equation in both finite and periodic systems. The proposed method features a robust and systematically convergent design, while significantly reducing the degrees of freedom compared with traditional finite element schemes. Numerical experiments are conducted to illustrate the accuracy and efficiency.

个人简介:蔡泽宇,中国科学技术大学数学科学学院博士研究生,导师为徐岩教授,主要研究方向为计算与应用数学。主要关注密度泛函理论的全电子计算及其数值离散方法,近期致力于发展基于间断伽辽金框架的全电子科恩-沈方程高效求解算法,提升计算精度与可扩展性。希望通过本次研讨会与来自全国的青年学者交流在数值分析与电子结构计算中的前沿问题,拓宽研究视野、提升科研能力。

#### 时空一致高效高精度的 DG-HGKS 算法研究

#### 张梦晴

#### 北京应用物理与计算数学研究所

本报告提出了一种时空一致的高效高精度间断有限元气体动理学格式(DG-HGKS),用于求解可压缩流动的欧拉方程。该格式具有以下特点:

一方面,DG-HGKS 是紧致高效高阶气体动理学格式(CEHGKS,Li et al., 2021,JCP.) 的拓展。其核心思想包括两个部分: 首先,从全离散的 DG 格式出发,对数值通量和体积分进行时间上的泰勒展开; 其次,借鉴 CEHGKS 中的技术,将时间导数替换为空间导数。为了在间断区域有效抑制非物理振荡,并最大限度地减少"问题单元"的数量,本研究结合了 KXRCF 探测器和 SHWENO 重构技术,开发了一种与新格式兼容的有效限制器策略。该格式能够在空间和时间上实现任意高阶精度,突破了现有单步 DG-HGKS 精度不超过三阶的限制。

另一方面,将上述基于全局时间步进(GTS)框架下 DG-HGKS 格式推广到局部时间步进(LTS)框架下,发展了一种更加高效的算法。其核心思想在于允许计算单元根据局部 CFL 稳定性条件采用不同的时间步长。LTS 算法避免了GTS 中最严格 CFL 条件的限制,在保持良好数值结果的同时提升了计算效率。此外,首次将 LTS 技术引入 DG-HGKS 方法中,为复杂流体力学问题的求解提供了更为高效的数值工具。

一维及二维典型算例验证了算法的鲁棒性、高阶精度及计算效率优势。

个人简介: 张梦晴,就读于北京应用物理与计算数学研究所,2022 级博士研究生,导师为陈艺冰研究员。主要研究方向为计算流体力学的时空一致高精度算法,重点聚焦于间断有限元的气体动理学方法。目前科研成果以第一作者身份向《Journal of Computational Physics》期刊投稿一篇,一篇正在撰写。多次参加学术交流会议,2024年10月于南京参加中国工业与应用数学学术年会(CSIAM2024)并作专题报告;2025年5月于南昌参加第二届魅丽数学与交叉应用会议并墙报展示,且荣获墙报优秀奖。在学业上连续三年获得中物院研究生"一等学业奖学金"。

# A third-order structure-preserving exponential time differencing Runge-Kutta scheme for the binary fluid-surfactant phase field model

#### 段嘉怡

#### 香港理工大学

In this talk, we present a third-order (in time) numerical scheme for a binary fluidsurfactant phase field model which consists of two coupled Cahn-Hilliard type equations. The proposed scheme inherits the structure-preserving property of the model, including energy dissipation and bound preservation. To maintain the dissipation with respect to the original free energy, a linear convex splitting of the energy functional is first introduced. The numerical scheme is then developed by employing a spectral collocation approximation for spatial discretization and a third-order exponential time differencing Runge-Kutta scheme for time integration. Benefiting from the explicit evaluations of the nonlinear and coupling terms, the proposed scheme is linear and completely decoupled. By treating the numerical solution as the sum of the exact solution and a small perturbation, the bound-preserving property of the proposed scheme is proved concomitant with its convergence. The original energy dissipation is further achieved with the help of the convex splitting method and the controlling of the nonlinear and coupling terms. Some numerical experiments in two and three dimensions are performed to verify the theoretical results and demonstrate the efficiency of the proposed scheme for simulations of phase separation phenomena.

Short Bio: Ms. Jiayi Duan obtained her Bachelor's degree from Zhengzhou University in 2022 and is currently a PhD student in the Department of Applied Mathematics at The Hong Kong Polytechnic University, under the supervision of Prof. Zhonghua Qiao. Ms. Duan's research focuses on scientific computing and numerical analysis for phase field equations.

# Energy stable finite element approximations of gas flow in poroelastic media

#### 陈玉祥

#### 厦门大学

We present energy-stable numerical methods for modeling gas flow in porous media, considering full compressibility. Our key innovation is a reformulation using the chemical potential gradient as the driving force, which naturally satisfies energy dissipation. The proposed numerical scheme combines a semi-implicit time discretization with discontinuous Galerkin and mixed finite element methods. This approach preserves mass conservation and energy dissipation at the discrete level, while maintaining density boundedness. Numerical experiments demonstrate the method's accuracy and robustness in handling strong nonlinear coupling, providing an effective tool for simulating complex porous media flows.

个人简介: 陈玉祥,厦门大学博士研究生在读,研究内容涉及多孔介质中流动与输运问题的数值方法研究,主要聚焦于数学建模和高效算法设计,目前已在计算数学领域著名期刊,《Journal of Scientific Computing》和《Computer Methods in Applied Mechanics and Engineering》上发表了多篇学术论文。

### A space-decoupling framework for optimization on boundedrank matrices with orthogonally invariant constraints

#### 杨俨

#### 中国科学院数学与系统科学研究院

Imposing additional constraints on low-rank optimization has garnered growing interest recently. However, the geometry of coupled constraints restricts the well-developed low-rank structure and makes the problem nonsmooth. In this paper, we propose a space-decoupling framework for optimization problems on bounded-rank matrices with orthogonally invariant constraints. The "space-decoupling" is reflected in several ways. Firstly, we show that the tangent cone of coupled constraints is the intersection of the tangent cones of each constraint. Secondly, we decouple the intertwined bounded-rank and orthogonally invariant constraints into two spaces, resulting in optimization on a smooth manifold. Thirdly, we claim that implementing Riemannian algorithms is painless as long as the geometry of additional constraint is known a priori. In the end, we unveil the equivalence between the original problem and the reformulated problem. The numerical experiments validate the effectiveness and efficiency of the proposed framework.

个人简介:杨俨,中国科学院数学与系统科学研究院直博四年级研究生,师从袁亚湘研究员。主要研究方向为低秩优化与双层优化。他在双层优化方面的研究成果已发表在人工智能顶级会议 ICLR 和 AISTATS 上,低秩优化的系列工作也已投稿至优化领域权威期刊。

# RiNNAL+: a Riemannian ALM Solver for SDP-RLT Relaxations of Mixed-Binary Quadratic Programs

#### 侯頔

#### 新加坡国立大学

Doubly nonnegative (DNN) relaxation usually provides a tight lower bound for a mixed-binary quadratic program (MBQP). However, solving DNN problems is challenging because: (1) the problem size is  $\Omega((n + \ell)^2)$  for an MBQP with n variables and  $\ell$  inequality constraints, and (2) the rank of optimal solutions cannot be estimated a priori due to the absence of theoretical bounds. In this work, we propose RiNNAL+, a Riemannian augmented Lagrangian method (ALM) for solving DNN problems. We prove that the DNN relaxation of an MBQP, with matrix dimension  $(n + \ell + 1)$ , is equivalent to the SDP-RLT relaxation (based on the reformulation-linearization technique) with a smaller matrix dimension (n + 1). In addition, we develop a hybrid method that alternates between two phases to solve the ALM subproblems. In phase one, we apply low-rank matrix factorization and random perturbation to transform the feasible region into a lower-dimensional manifold so that we can use the Riemannian gradient descent method. In phase two, we apply a single projected gradient step to update the rank of the underlying variable and escape from spurious local minima arising in the first phase if necessary. To reduce the computation cost of the projected gradient step, we develop pre-processing and warm-start techniques for acceleration. Unlike traditional rank-adaptive methods that require extensive parameter tuning, our hybrid method requires minimal tuning. Extensive experiments confirm the efficiency and robustness of RiNNAL+ in solving various classes of large-scale DNN problems.

个人简介:侯頔,现为新加坡国立大学数学专业博士研究生,导师为 Toh Kim-Chuan 教授。2022 年本科毕业于吉林大学唐敖庆理科试验班。研究方向包括矩阵优化,半定规划的算法设计及其应用。相关工作发表在 Operations Research 等期刊。

# Backward analysis of the total least squares and its randomized algorithms

#### 单佳骊

#### 复旦大学

Total least squares (TLS), an extension to the well-known least squares (LS), merits the specific problem structure that takes errors in all variables into consideration and thus is closer to the real-world situation. However, solving large-scale or ill-conditioned TLS systems are computationally prohibitive and most existing algorithms lack stability.

In this talk, TLS is accessed through the lens of backward error analysis and a new fast TLS solver is designed. We originally derive the explicit expression for the optimal backward error of the general multidimensional total least squares (mTLS) problem, with both full-rank and rank-deficient computed solutions considered. In order to facilitate practical computation, we further propose an estimate for the single right-hand side case with a very tight bound and provide a better routine to solve the multidimensional one where randomization is exploited. Theoretical results reveal deep connections between the LS and the TLS. Finally, we will present a fast randomized TLS algorithm which is based on the Rayleigh Quotient Iteration framework and proved to maintain the convergence rate.

个人简介:单佳骊,复旦大学数学科学学院博士研究生。主要研究方向为随机数值线性代数,重点关注整体最小二乘系统的理论分析与实际应用,研究 其误差分析及面向大规模科学计算问题的快速稳定数值方法。曾参与国家自然 科学基金青年学者基础研究项目,并赴加州大学伯克利分校访学。

### A Simplified Algorithm for Joint Real-Time Synchronization, NLoS Identification, and Multi-Agent Localization

#### 邓一理

#### 清华大学

Real-time, high-precision localization in large-scale wireless networks faces two primary challenges: clock offsets caused by network asynchrony and non-line-of-sight (NLoS) conditions. To tackle these challenges, we propose a low-complexity real-time algorithm for joint synchronization and NLoS identification-based localization. For precise synchronization, we resolve clock offsets based on accumulated time-of-arrival measurements from all the past time instances, modeling it as a large-scale linear least squares (LLS) problem. To alleviate the high computational burden of solving this LLS, we introduce the blockwise recursive Moore-Penrose inverse (BRMP) technique, a generalized recursive least squares approach, and derive a simplified formulation of BRMP tailored specifically for the real-time synchronization problem. Furthermore, we formulate joint NLoS identification and localization as a robust least squares regression (RLSR) problem and address it by using an efficient iterative approach. Simulations show that the proposed algorithm achieves sub-nanosecond synchronization accuracy and centimeter-level localization precision, while maintaining low computational overhead.

个人简介: 邓一理,清华大学数学科学系,研究方向为无线信号处理中相关优化问题的建模、求解与算法加速。希望和大家深入交流,探讨数学与无线的交叉问题。

# Interference-Free Propagation: Achieving Reliable Signal Propagation in Brain Networks with Areal-Specific Local Dynamics

#### 金振远

#### 上海交通大学

Many complex networks are able to propagate signals reliablely while maintaining node-specific local dynamics. However, the underlying mechanism remains largely unclear. In general, strong connections between nodes enhance signal propagation but blend timescales of node-specific local activity, while weak connections have the opposite effect. We identify a novel dynamical regime termed "interference-free propagation" (IFP) that reconciles the two contrasting demands both in a multi-area spiking neural network and in a rate-based model. In the IFP regime, mean signals from upstream nodes can propagate reliably but fluctuations indicative of upstream nodes' timescales are filtered out. This result provides new insights into the operational regime of complex networks like the brain, leading to the coexistence of reliable signal propagation and the distinct property of local temporal integration of information.

Short Bio: Zhenyuan Jin is currently a doctoral candidate in the School of Mathematical Sciences, Shanghai Jiao Tong University, under the supervision of Professor Songting Li and Douglas Zhou. His research focuses on two interconnected themes: the modeling of brain networks based on spatial geometric structures and the analysis of spiking neural network models. The primary objective of his work is to leverage rigorous mathematical frameworks to elucidate fundamental neural mechanisms.

### A singularity guided Nyström method for 2D elastostatics with corners

#### 谢宝玲

#### 浙江大学

Corner singularities fundamentally limit the accuracy and stability of boundary integral formulations for the 2D Lamé system on cornered domains. This talk develops a paired theory-algorithm framework. First, a local Mellin analysis on a wedge yields a factorizable characteristic equation for the density's singular exponents, cleanly separating physical branches and explaining their dependence on opening angle and boundary conditions. In weighted Sobolev spaces, we establish a Fredholm well-posedness criterion for the interior double-layer equation by excluding a computable discrete set on the critical line, and construct an explicit density-to-Taylor mapping that is invertible for all but countably many angles. Guided by these results, we design a singularity-guided Nyström (SGN) scheme: corner exponents drive panel adaptivity via a multi-exponent Legendre-tail indicator, while near and self interactions are handled by a forward-stable Cauchy-Legendre recurrence. Numerical tests on convex and reentrant corners show clear accuracy gains over uniform Nyström and reveal a crowding-limited regime at re-entrant angles.

Short Bio: Baoling Xie is a Ph.D. student in Computational Mathematics at the School of Mathematical Sciences, Zhejiang University, advised by Prof. Jun Lai. Her research focuses on high-accuracy numerical algorithms for PDEs, including boundary integral equations, corner singularities, and computational physics problems such as high-resolution imaging and resonance phenomena. Her recent work develops corner spectra and singularity-guided Nyström methods for 2D elastostatics, combining Mellin-symbol analysis with an adaptive high-order solver.

# Stability Analysis of Monolithic Globally Divergence-Free ALE-HDG Methods for Fluid-Structure Interaction

#### 刘帅军

#### 四川大学

We propose two monolithic arbitrary order finite element schemes for fluid-structure interaction (FSI), based on a novel Piola-type Arbitrary Lagrangian-Eulerian (ALE) mapping, and analyze the stability of these schemes. For temporal discretization, we first derive the discrete geometric conservation law (GCL) and then apply the backward Euler method to both the non-conservative and conservative formulations. We examine the connection between the stability of the backward Euler scheme and the fulfillment of the discrete GCL condition in H(div)-conforming methods for FSI problems. For spatial discretization, we adopt hybridizable discontinuous Galerkin (HDG) methods for the incompressible Navier-Stokes and linear elasticity equations, and a continuous Galerkin (CG) method for mesh movement. Owing to the use of discontinuous spaces k/k for velocity and its trace, and k-1/k for pressure and its trace, we further prove that the velocity approximation is globally divergence-free. We also present numerical experiments demonstrating the effectiveness of the proposed methods.

个人简介: 刘帅军,四川大学数学学院 2023 级博士研究生,导师谢小平教授,主要研究方向为有限元方法及其在流体力学、磁流体力学与流固耦合问题中的数值模拟与分析。研究重点包括保持散度约束的高精度有限元离散方法、杂交间断有限元(HDG)方法、任意拉格朗日-欧拉(ALE)框架下的动网格数值算法及稳定性与收敛性分析。

### Error estimates of the Strang splitting scaled Laguerre--Fourier pseudospectral method for the Gross--Pitaevskii equation with angular momentum rotation

#### 李英恺

#### 北京师范大学

In this paper, we show that the scaled Laguerre--Fourier interpolation can be interpreted as a weighted least squares approximation in a discrete inner product space, and we provide a detailed analysis of its approximation properties. Building on this foundation, we conduct a rigorous convergence analysis of Strang splitting scheme combined with the scaled Laguerre--Fourier interpolation for the Gross--Pitaevskii equation (GPE) with angular momentum rotation. Our analysis establishes that the numerical scheme achieves second-order accuracy in time and spectral accuracy in space under suitable regularity assumptions. Numerical experiments are presented to validate the theoretical results and to illustrate the accuracy and efficiency of the method.

个人简介:李英恺,北京师范大学数学科学学院,计算数学方向 2024 级博士生,导师为蔡勇勇教授。主要研究方向为玻色爱因斯坦凝聚态的基态解及动力学数值计算、谱方法与误差分析、Gross-Pitaevskii 方程的保结构算法等。

### 会议记录

### 会议记录