北京理工大學

数学与统计学院学术报告

A Damped Subspace Splitting Algorithm for Constrained Density Functional Theory



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摘 要 ： Constrained density functional theory (CDFT) provides a powerful framework for describing electronically excited and charge-localized states, which underlie a broad range of physical and chemical phenomena. However, the discretized optimization problems arising from CDFT calculations remain challenging, owing to the presence of both the Stiefel manifold constraint and additional nonconvex quadratic constraints. Existing algorithms either fail to enforce the quadratic constraints with high accuracy or face convergence issues due to double-loop iterative structures. In this paper, we first derive a subspace-splitting reformulation that decouples the two groups of constraints, by exploiting the inherent rotation invariance and introducing a nonlinear subspace alignment constraint. Based on this reformulation, we propose a single-loop damped alternating direction method of multipliers, called DASSP. To the best of our knowledge, DASSP is the first algorithm for CDFT calculations with rigorous convergence guarantees. Each iteration of DASSP comprises a spectral minimization step, a projected gradient step, and a damped dual ascent step, all of which admit efficient implementations. Numerical results on synthetic and realistic CDFT problems demonstrate that DASSP attains high feasibility accuracy and exhibits favorable efficiency without compromising robustness. We expect that this work will pave the way toward reliable and efficient large-scale CDFT applications.

报告人简介： 刘歆，中国科学院数学与系统科学研究院研究员，博士生导师，计算数学与科学工程计算研究所副所长。主要研究方向包括流形优化、分布式优化及其在材料计算、大数据分析和机器学习等领域的应用。刘歆分别于2016年，2021年和2023年获得国家自然科学基金委优秀青年科学基金项目、杰出青年科学基金项目和科技部重点专项的资助。2024年获得中国工业与应用数学学会萧树铁应用数学奖，2026年当选中国工业与应用数学学会会士。现担任MPC，JCM，APJOR等国内外期刊编委，《中国科学 · 数学》（中英文）青年编委，《计算数学》副主编；中国科学院青年创新促进会理事长；中国工业与应用数学学会秘书长、优化及其应用专业委员会主任；中国运筹学会常务理事；中国数学会计算数学分会常务理事。

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