DENSITY MATRIX MINIMIZATION WITH ℓ_1 REGULARIZATION *

RONGJIE LAI†, JIANFENG LU‡, AND STANLEY OSHER§

Abstract. We propose a convex variational principle to find sparse representation of low-lying eigenspace of symmetric matrices. In the context of electronic structure calculation, this corresponds to a sparse density matrix minimization algorithm with ℓ_1 regularization. The minimization problem can be efficiently solved by a split Bregman iteration type algorithm. We further prove that from any initial condition, the algorithm converges to a minimizer of the variational principle.

Key words. Density matrix, ℓ_1 regularization, eigenspace

AMS subject classifications. 65K10, 65F30

1. Introduction

The low-lying eigenspace of operators has many important applications, including those in quantum chemistry, numerical PDEs, and statistics. Given a $n \times n$ symmetric matrix H, and denote its eigenvectors as $\{\Phi_i\}, i = 1, \ldots, n$. The low-lying eigenspace is given by the span of the first N (usually $N \ll n$) eigenvectors.

In many scenario, the real interest is the subspace itself, but not a particular set of basis functions. In particular, we are interested in a sparse representation of the eigenspace. The eigenvectors forms a natural basis set, but for oftentimes they are not sparse or localized (consider for example the eigenfunctions of the free Laplacian operator $-\Delta$ on a periodic box). This suggests asking for an alternative sparse representation of the eigenspace.

In quantum chemistry, the low-lying eigenspace for a Hamiltonian operator corresponds to the physically occupied space of electrons. In this context, a localized class of basis functions of the low-lying eigenspaces is called Wannier functions [14, 28]. These functions provide transparent interpretation and understandings of covalent bonds, polarizations, etc. of the electronic structure. These localized representations are also the starting point and the essence for many efficient algorithms for electronic structure calculations (see e.g. the review article [10]).

1.1. Our contribution

In this work, we propose a convex minimization principle for finding a sparse representation of the low-lying eigenspace.

$$\min_{P \in \mathbb{R}^{n \times n}} \ \operatorname{tr}(HP) + \frac{1}{\mu} \|P\|_1,$$
$$\text{s.t.} \ P = P^{\mathrm{T}}, \operatorname{tr} P = N, 0 \preceq P \preceq I. \tag{1.1}$$

where $\|\cdot\|_1$ is the entrywise ℓ_1 matrix norm, $A \preceq B$ denotes that $B - A$ is a positive semi-definite matrix, and μ is a penalty parameter for entrywise sparsity. Here H

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Density Matrix Minimization With Regularization

Michele Benzi,Dario Bini,Daniel Kressner,Hans Munthe-Kaas,Charles Van Loan

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Exploiting Hidden Structure in Matrix Computations: Algorithms and Applications Michele Benzi,Dario Bini,Daniel Kressner,Hans Munthe-Kaas,Charles Van Loan,2017-01-24 Focusing on special matrices and matrices which are in some sense near to structured matrices this volume covers a broad range of topics of current interest in numerical linear algebra Exploitation of these less obvious structural properties can be of great importance in the design of efficient numerical methods for example algorithms for matrices with low rank block structure matrices with decay and structured tensor computations Applications range from quantum chemistry to queuing theory Structured matrices arise frequently in applications Examples include banded and sparse matrices Toeplitz type matrices and matrices with semi separable or quasi separable structure as well as Hamiltonian and symplectic matrices The associated literature is enormous and many efficient algorithms have been developed for solving problems involving such matrices The text arose from a C I M E course held in Cetraro Italy in June 2015 which aimed to present this fast growing field to young researchers exploiting the expertise of five leading lecturers with different theoretical and application perspectives **High-Performance Tensor Computations in Scientific Computing and Data Science** Edoardo Angelo Di Napoli,Paolo Bientinesi,Jiajia Li,André Uschmajew,2022-11-08 **Mathematical Methods in Engineering** Nuno Miguel Fonseca Ferreira,José António Tenreiro Machado,2014-08-18 This book presents a careful selection of the contributions presented at the Mathematical Methods in Engineering MME10 International Symposium held at the Polytechnic Institute of Coimbra Engineering Institute of Coimbra IPC ISEC Portugal October 21 24 2010 The volume discusses recent developments about theoretical and applied mathematics toward the solution of engineering problems thus covering a wide range of topics such as Automatic Control Autonomous Systems Computer Science Dynamical Systems and Control Electronics Finance and Economics Fluid Mechanics and Heat Transfer Fractional Mathematics Fractional Transforms and Their Applications Fuzzy Sets and Systems Image and Signal Analysis Image Processing Mechanics Mechatronics Motor Control and Human Movement Analysis Nonlinear Dynamics Partial Differential Equations Robotics Acoustics Vibration and Control and Wavelets *The Magnetotelluric Method* Alan D. Chave,Alan G. Jones,2012-04-26 The magnetotelluric method is a technique for imaging the electrical conductivity and structure of the Earth from the near surface down to the 410 km transition zone and beyond This book forms the first comprehensive overview of magnetotellurics from the salient physics and its mathematical representation to practical implementation in the field data processing modeling and geological interpretation Electromagnetic induction in 1 D 2 D and 3 D media is explored building from first principles and with thorough coverage of the practical techniques of time series processing distortion numerical modeling and inversion The fundamental principles are illustrated with a series of case histories describing geological applications Technical issues instrumentation and field practices are described for both land and marine surveys This book provides a rigorous introduction to magnetotellurics for academic researchers and advanced

students and will be of interest to industrial practitioners and geoscientists wanting to incorporate rock conductivity into their interpretations **Elements of Quantum Information** Wolfgang P. Schleich,Herbert Walther,2007-06-27 Elements of Quantum Information introduces the reader to the fascinating field of quantum information processing which lives on the interface between computer science physics mathematics and engineering This interdisciplinary branch of science thrives on the use of quantum mechanics as a resource for high potential modern applications With its wide coverage of experiments applications and specialized topics all written by renowned experts Elements of Quantum Information provides an indispensable up to date account of the state of the art of this rapidly advancing field and takes the reader straight up to the frontiers of current research The articles have first appeared as a special issue of the journal Fortschritte der Physik Progress of Physics Since then they have been carefully updated The book will be an inspiring source of information and insight for anyone researching and specializing in experiments and theory of quantum information **Formulation and Numerical Solution of Quantum Control Problems** Alfio Borzi,Gabriele Ciaramella,Martin Sprengel,2017-07-06 This book provides an introduction to representative nonrelativistic quantum control problems and their theoretical analysis and solution via modern computational techniques The quantum theory framework is based on the Schr dinger picture and the optimization theory which focuses on functional spaces is based on the Lagrange formalism The computational techniques represent recent developments that have resulted from combining modern numerical techniques for quantum evolutionary equations with sophisticated optimization schemes Both finite and infinite dimensional models are discussed including the three level Lambda system arising in quantum optics multispin systems in NMR a charged particle in a well potential Bose Einstein condensates multiparticle spin systems and multiparticle models in the time dependent density functional framework This self contained book covers the formulation analysis and numerical solution of quantum control problems and bridges scientific computing optimal control and exact controllability optimization with differential models and the sciences and engineering that require quantum control methods *Journal of Propulsion and Power* ,2008 *Big Data Analysis* Junwei Lu,2025-12-07 This book covers the methods and theory of high dimensional probability statistics large scale optimization and inference We aim to quickly bring readers to the frontier and interdisciplinary areas of statistics optimization probability and machine learning This book covers topics in High dimensional probability Concentration inequality Sub Gaussian random variables Chernoff bounds Hoeffding s inequality Maximal inequalities High dimensional linear regression Ordinary least square Compressed sensing Lasso Variations of Lasso including group lasso fused lasso adaptive lasso etc General high dimensional M estimators Variable selection consistency High dimensional Optimization Convex geometry Lagrange duality Gradient descent Proximal gradient descent LARS ADMM Mirror descent Stochastic optimization Large Scale Inference Linear model hypothesis testing high dimensional inference Chi square test maximal test and Higher criticism False discovery rate control **Brain Source Localization Using EEG Signal Analysis** Munsif Ali

Jatoi,Nidal Kamel,2017-12-14 Of the research areas devoted to biomedical sciences the study of the brain remains a field that continually attracts interest due to the vast range of people afflicted with debilitating brain disorders and those interested in ameliorating its effects To discover the roots of maladies and grasp the dynamics of brain functions researchers and practitioners often turn to a process known as brain source localization which assists in determining the source of electromagnetic signals from the brain Aiming to promote both treatments and understanding of brain ailments ranging from epilepsy and depression to schizophrenia and Parkinson s disease the authors of this book provide a comprehensive account of current developments in the use of neuroimaging techniques for brain analysis Their book addresses a wide array of topics including EEG forward and inverse problems the application of classical MNE LORETA Bayesian based MSP and its modified version M MSP Within the ten chapters that comprise this book clinicians researchers and field experts concerned with the state of brain source localization will find a store of information that can assist them in the quest to enhance the quality of life for people living with brain disorders   Advances in Geophysics Bimalendu Bhusan Bhattacharya,1988 Contributed articles   Journal of Thermophysics and Heat Transfer ,1989   Radio Science ,2008   **Biomag 2004** Eric Halgren,2004   **Inverse Methods** Bo Holm Jacobsen,Klaus Mosegaard,1996-09-18 Over the last few decades inversion concepts have become an integral part of experimental data interpretation in several branches of science In numerous cases similar inversion like techniques were developed independently in separate disciplines sometimes based on different lines of reasoning but not always to the same level of sophistication This book is based on the Interdisciplinary Inversion Conference held at the University of Aarhus Denmark For scientists and graduate students in geophysics astronomy oceanography petroleum geology and geodesy the book offers a wide variety of examples and theoretical background in the field of inversion techniques   Lithuanian Physics Journal ,1997   *Annales Geophysicae* ,2009 An international multi and interdisciplinary scientific journal of original articles and of short communications in the following fields physics and dynamics of the oceans and seas incl oceanography and marine sciences air sea and air land vegetation interactions incl physical chemical and biological processes modelling and remote sensing of oceans atmospheres and climate physics dynamics and chemistry of the lower middle and upper atmosphere of the Earth incl meteorology and climatology physics of ionosphere and magnetosphere of the Earth incl solarterrestrial relations geomagnetism and magnetic activity interplanetary and heliospheric physics incl solar wind energetic particles and radiation belts of the Earth physics and dynamics of the solar atmosphere incl chromosphere and corona emissions and magnetic activity space plasma physics and active experiments in space   *Journal of the American Statistical Association* ,2009   **Expanded Abstracts with Biographies** ,2003   **Handbook of Surfaces and Interfaces of Materials: Surface and interface analysis and properties** Hari Singh Nalwa,2001   **Journal of the Optical Society of America** ,2006

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