

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 $\{\Phi_i\}_{i=1, \dots, n}$. 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 form 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.

$$\begin{aligned} \min_{P \in \mathbb{R}^{n \times n}} \quad & \text{tr}(HP) + \frac{1}{\mu} \|P\|_1 \\ \text{s.t.} \quad & P = P^T, \text{tr}P = N, 0 \leq P \leq I, \end{aligned} \tag{1.1}$$

where $\|\cdot\|_1$ is the entrywise ℓ_1 matrix norm, $A \leq B$ 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:

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

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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

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