

# DENSITY MATRIX MINIMIZATION WITH $\ell_1$ REGULARIZATION \*

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**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  $\ell_1$  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,  $\ell_1$  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  $\ell_1$  matrix norm,  $A \leq B$  denotes that  $B - A$  is a positive semi-definite matrix, and  $\mu$  is a penalty parameter for entrywise sparsity. Here  $H$

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# Density Matrix Minimization With Regularization

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## **Table of Contents Density Matrix Minimization With Regularization**

1. Understanding the eBook Density Matrix Minimization With Regularization
  - The Rise of Digital Reading Density Matrix Minimization With Regularization
  - Advantages of eBooks Over Traditional Books
2. Identifying Density Matrix Minimization With Regularization
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Density Matrix Minimization With Regularization
  - User-Friendly Interface
4. Exploring eBook Recommendations from Density Matrix Minimization With Regularization
  - Personalized Recommendations

- Density Matrix Minimization With Regularization User Reviews and Ratings
- Density Matrix Minimization With Regularization and Bestseller Lists
- 5. Accessing Density Matrix Minimization With Regularization Free and Paid eBooks
  - Density Matrix Minimization With Regularization Public Domain eBooks
  - Density Matrix Minimization With Regularization eBook Subscription Services
  - Density Matrix Minimization With Regularization Budget-Friendly Options
- 6. Navigating Density Matrix Minimization With Regularization eBook Formats
  - ePub, PDF, MOBI, and More
  - Density Matrix Minimization With Regularization Compatibility with Devices
  - Density Matrix Minimization With Regularization Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Density Matrix Minimization With Regularization
  - Highlighting and Note-Taking Density Matrix Minimization With Regularization
  - Interactive Elements Density Matrix Minimization With Regularization
- 8. Staying Engaged with Density Matrix Minimization With Regularization
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Density Matrix Minimization With Regularization
- 9. Balancing eBooks and Physical Books Density Matrix Minimization With Regularization
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Density Matrix Minimization With Regularization
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Density Matrix Minimization With Regularization
  - Setting Reading Goals Density Matrix Minimization With Regularization
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Density Matrix Minimization With Regularization
  - Fact-Checking eBook Content of Density Matrix Minimization With Regularization

- Distinguishing Credible Sources
- 13. Promoting Lifelong Learning
  - Utilizing eBooks for Skill Development
  - Exploring Educational eBooks
- 14. Embracing eBook Trends
  - Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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