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 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.

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

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:

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