
Density Matrix Minimization With Regularization

Density Matrix Minimization With Regularization - [Free] *Density Matrix Minimization With Regularization* [PDF] [EPUB] arXiv:1403.1525v1 [math-ph] 6 Mar 2014 DENSITY MATRIX MINIMIZATION WITH ℓ_1 REGULARIZATION RONGJIELAI, 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. Type. Journal article. Permalink ... Density matrix minimization with ℓ_1 regularization 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. Orbital Minimization Method with ℓ_1 Regularization - samsi.info Orbital Minimization Method with ℓ_1 Regularization Jianfeng Lu and Kyle Thicke Duke University, Math Department Main Points •Used ℓ_1 regularization and the sparsity to compute localized density matrices for both zero temperature and finite temperature cases, by adding an entry-wise ℓ_1 regularization to the free energy of the quantum system.

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