Density Matrix Minimization With Regularization

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Density Matrix Minimization With Regularization

DENSITY MATRIX MINIMIZATION WITH ℓ1 REGULARIZATION RONGJIELAI, JIANFENG LU,ANDSTANLEYOSHER 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 ℓ1

DENSITY MATRIX MINIMIZATION WITH REGULARIZATION

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...

(PDF) Density matrix minimization with l1 regularization

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...

Density matrix minimization with ${\ell}_1$ regularization

In the context of electronic structure calculation, this corresponds to a sparse density matrix minimization algorithm with ℓ1 regularization. The minimization problem can be efficiently solved by a split Bregman iteration type algorithm.

Density matrix minimization with ℓ1 regularization

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[1403.1525] Density matrix minimization with $\ell_1 ...

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Density matrix minimization with ℓ_1 regularization

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Density Matrix Minimization With Regularization

Note that it is possible to lift the orthogonality constraint by convexification, as in , , which leads to localized density matrix minimization. However, the density matrix P ∈ C N ×

N, which is the projection operator onto the low-lying eigenspace, contains many more degrees of freedom than X when N ≫ m.

Orbital minimization method with ℓ1 regularization ...

A density matrix is a matrix that describes the statistical state, whether pure or mixed, of a system in quantum mechanics.The probability for any outcome of any well-defined measurement upon a system can be calculated from the density matrix for that system. The extreme points in the set of density matrices are the pure states, which can also be written as state vectors or wavefunctions.

Density matrix - Wikipedia

Based on the fact that the density matrix decays exponentially away from the diagonal for insulating systems or systems at finite temperature, the proposed ℓ 1 regularized variational method provides an effective way to approximate the original quantum system.

Localized density matrix minimization and linear-scaling ...

To well address the problem of noise and outliers, it imposes joint L2,1 -norm minimization on both the loss function of NMF and the regularization of the basis matrix. The geometric structure and the joint L2,1 -norm are formulated as an optimization model, which is solved by the proposed iterative algorithm.

Robust nonnegative matrix factorization with structure ...

Tikhonov regularization addresses the numerical insta-bility of the matrix inversion and subsequently produces lower variance models. This method adds a positive con-stant to the diagonals of XT X, to make the matrix non-singular [2]. The analytic solution then becomes: w = (XT X +,I)i1XT y (7) If we replace one diagonal value of the I ...

Least Squares Optimization with L1-Norm Regularization

Kohn–Sham density functional theory (DFT) is the most widely used electronic structure theory. Despite significant progress in the past few decades, the numerical solution of Kohn–Sham DFT problems remains challenging, especially for large-scale systems.

Numerical methods for Kohn–Sham density functional theory ...

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Localized density matrix minimization and linear-scaling ...

a structured matrix rank minimization problem. There are several other applications where such linear structure is of great importance—see e.g., [11] and references therein. Furthermore, since (enhanced) structured matrix completion also falls into the category of rank minimization problems,

Efficient Structured Matrix Rank Minimization

R. Lai, J. Lu, “Localized Density Matrix Minimization and Linear Scaling Algorithms”, 315, pp. 194–210, Journal of Computational Physics, 2016. ... R. Lai, J. Li, “Manifold Based Low-rank Regularization for Image Restoration and Semi-supervised Learning”, Journal of Scientific Computing, 74(3), pp 1241–1263, 2018.

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