Weighted Trace-Penalty Minimization for Full Configuration Interaction

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Abstract: To solve the linear Hermitian extreme eigenpairs problem arising from the Full Configuration Interaction (FCI) method in electronic structure calculation, an unconstrained optimization model called weighted trace-penalty minimization is proposed. The main results that the corresponding global minimizers are the blocks of eigenvectors instead of invariant subspace indicates that the cost of orthonormalization or Rayleigh-Ritz process could be saved. Due to the characteristics of extremely large scale and "sparsity" of eigenvectors, solving the minimization problem by the coordinate descent algorithm accelerates the convergence and saves the storage of data in comparison with the gradient methods, making the cost affordable.