Optimization Based Approaches for Partial Eigenvalue Decomposition

X. Liu[1]

Abstract: In a block algorithm for computing a relatively high-dimensional eigenspaces of large sparse symmetric matrices, the Rayleigh-Ritz (RR) procedure often constitutes a major bottleneck. Although dense eigenvalue calculations for subproblems in RR steps can be parallelized to a certain level, their parallel scalability, which is limited by some inherent sequential steps, is lower than dense matrix-matrix multiplications. The primary motivation of this paper is to develop a methodology that reduces the use of the RR procedure in exchange for matrix-matrix multiplications. We propose two unconstrained trace-penalty minimization models and establish their equivalence to the eigenvalue problem. It enable us to deploy algorithms for calculating eigenspace by soling either of these two special unconstrained optimization models. Although the proposed algorithms do not necessarily reduce the total number of arithmetic operations, they leverage highly optimized operations on modern high performance computers to achieve parallel scalability. Numerical results based on a preliminary implementation, parallelized using OpenMP, show that our approaches are promising.

[1] State Key Laboratory of Scientific and Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences
55. Zhong Guan Cun East Road, Beijing, 100190, China
liuxin@lsec.cc.ac.cn