数学与系统科学研究院

计算数学所定期学术报告

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报告题目:

Block algorithms with augmented Rayleigh-Ritz projections for large-scale eigenpair computation

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<u>报告时间</u>: 2015 年 6 月 4 日 (周四) 下午 16:00~17:00

<u>报告地点</u>: 科技综合楼三层 311 报告厅

Abstract:

Iterative algorithms for computing eigenpairs of large matrices consist of two main steps: a subspace update step and a Rayleigh-Ritz (RR) step. In this paper, we propose an augmented Rayleigh-Ritz (ARR) step that can provably accelerate convergence under mild conditions. We consider two block (as opposed to Krylov subspace) algorithms by coupling the ARR procedure with two subspace update schemes: (i) the classic power method applied to multiple vectors without periodic orthogonalization, and (ii) a recently proposed Gauss-Newton method. In block algorithms, the RR step is arguably the bottleneck in scalability as the number of computed eigenpairs increases. Our key design objective is for the algorithms to approach a certain optimal scalability under favorable conditions. That is, to attain a sufficient accuracy, they should call the Rayleigh-Ritz step as few times as possible (ideally only once), while the subspace update step should be close to being embarrassingly parallel under suitable data mapping schemes. We perform extensive computational experiments in Matlab (without explicit code parallelization) to evaluate the proposed algorithms in comparison to a few state-of-the-art eigensolvers. Numerical results show strong potentials for the proposed algorithms to reach high levels of scalability on a representative set of test problems.

