ABSTRACT

The generalized eigenvalue problem is a fundamental numerical linear algebra problem whose applications are wide ranging. For truly large-scale problems, matrices themselves are often not directly accessible, but their actions as linear operators can be probed through matrix-vector multiplications. To solve such problems, matrix-free algorithms are the only viable option. In addition, algorithms that do multiple matrix-vector multiplications simultaneously (instead of sequentially), or so-called block algorithms, generally have greater parallel scalability that can prove advantageous on highly parallel, modern computer architectures.

In this work, we propose and study a new inverse-free, block algorithmic framework for generalized eigenvalue problems that is based on an extension of a recent framework called EIGPEN — an unconstrained optimization formulation utilizing the Courant Penalty function. We construct a method that borrows several key ideas, including projected gradient descent, back-tracking line search, and Rayleigh-Ritz (RR) projection. We establish a convergence theory for this framework.

We conduct numerical experiments to assess the performance of the proposed method in comparison to two well-known existing matrix-free algorithms, as well as to the popular solver ARPACK as a benchmark (even though it is not matrix-free). Our numerical results suggest that the new method is highly promising and worthy of further study and development.