
Orthogonalization Avoidant Davidson

Ioannis Thanasis*¹ and Erin C. Carson

¹Charles University – Czech Republic

Abstract

The Generalized-Davidson (GD) method is an iterative projection method used to compute eigenpairs of symmetric or Hermitian matrices. It constructs successive approximations of the wanted eigenpair by expanding an orthogonal basis using the preconditioned residual vector. In large-scale distributed computing environments, the frequent synchronizations required during orthogonalization can be a significant bottleneck. Moreover, the use of less expensive or approximate orthogonalization routines can significantly degrade accuracy or even lead to stagnation. In this work, we propose a synchronization avoiding reformulation of the GD method that eliminates the need for orthogonalization entirely by transforming the projected eigenvalue problem into a generalized eigenvalue problem. The method can be implemented with only a single global synchronization per iteration. We provide theoretical justification for this reformulation and present experimental results demonstrating its effectiveness and computational advantages.

*Speaker