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An implicit filter for rational Krylov using core transformations

Daan Camps *, Karl Meerbergen, Raf Vandebril

Department of Computer Science, KU Leuven – University of Leuven, Celestijnenlaan 200A, 3001 Leuven, Belgium

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ABSTRACT

The rational Krylov method is a powerful tool for computing a selected subset of eigenvalues in large-scale eigenvalue problems. In this paper we study a method to implicitly apply a filter in a rational Krylov iteration by directly acting on a QR factorized representation of the Hessenberg pair from the rational Krylov method. This filter is used to restart the iteration, which is generally required to limit the orthogonalization and storage costs. The contribution in this paper is threefold. We reformulate existing procedures in terms of operations on core transformations. This has the advantage of improved convergence monitoring. Secondly, we demonstrate that the extended QZ method is a special case of this more general method. Finally, numerical experiments show the validity and the increased accuracy of the new approach compared with existing methods.

* Corresponding author.
E-mail address: daan.camps@cs.kuleuven.be (D. Camps).

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1. Introduction

The Arnoldi algorithm, first introduced by Arnoldi (1951) [1] and studied extensively by Saad [2–5] is the *classical* Krylov method. It is a projection method frequently used for solving systems of linear equations, eigenvalue problems, matrix equations, and so forth. The Arnoldi algorithm generates a subspace on which the problem is projected. The resulting smaller problem is then solved, and lifted back to its original dimensions.

The Arnoldi method has a particular convergence behavior. If we focus on eigenvalue computations, it locates first well-separated extreme eigenvalues [5–7]. Computing, e.g., rightmost eigenvalues, eigenvalues near the origin or eigenvalues in a certain region with prescribed accuracy may be infeasible with a small number of Krylov vectors. One way to reduce the number of vectors is by using methods that converge faster towards a particular region of interest. *Shift-and-invert* Arnoldi [8–10] uses the matrix $(A - \sigma I)^{-1}$ to compute the eigenvalues near the 'shift' σ. In the rational Krylov method (RK), introduced by Ruhe [11–15], the shift or *pole* may change at every step in the iteration. The extended Krylov method (EK), first proposed by Druskin & Knizhnerman (1998) [16] for the approximation of matrix functions, is a special case of the RK method that only uses shifts at zero and infinity.

In every step of the Arnoldi algorithm, an explicit orthogonalization of the new vector against all previously computed basis vectors is performed. Consequently, the computational cost and storage requirements increase as the algorithm progresses. This problem can be solved by a restart of the Arnoldi method. Sorensen (1992) introduced the implicitly restarted Arnoldi method (IRA) [17]. His algorithm applies implicitly shifted QR steps on the Arnoldi Hessenberg matrix. The IRA method was further analyzed by Morgan (1996) [18] and refined by Lehoucq & Sorensen (1996) [19]. Stewart (2001) [20] introduced the Krylov–Schur algorithm where a proper subspace is extracted from the Krylov subspace via the Schur decomposition. De Samblanx, Meerbergen & Bultheel (1997) [21] proposed an implicit restart method for rational Krylov methods. Their method uses an explicit QZ step on the RK Hessenberg pencil. Recently, Berljafa & Güttel [22] proposed a method to change the poles in the RK method and noticed that this procedure can be used to restart the RK method [22, Section 4.3]. In their paper no comparison is made with the explicit method of De Samblanx et al. [21].

The contribution of this paper is threefold. First, we reformulate the method of Berljafa & Güttel in terms of operations on a QR-factorized representation of the RK Hessenberg pencil. In this representation, the unitary matrix is stored as a sequence of *core transformations*. This extends the *core chasing* techniques, introduced by Vandebril [23] for the dense eigenvalue problem and further developed by Vandebril & Watkins [24,25], beyond *condensed* matrices. As such it is effectively a reformulation of the rational QZ method [26] in terms of core transformations. This representation allows for an efficient storage scheme of the unitary matrices and admits an accurate deflation criterion [27]. Furthermore, we use this representation to study the structure of the projection