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Optimization of extrapolated Cayley transform with non-Hermitian positive definite matrix ☆

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For the extrapolated Cayley transform, we give necessary and sufficient conditions for guaranteeing its convergence and contraction (in the Euclidean norm). We derive upper bounds for the convergence and the contraction factors, and compute the optimal parameters minimizing these upper bounds and the corresponding optimal values of these upper bounds. Numerical computations show that these upper bounds are reasonably sharp compared with the exact convergence and the exact contraction factors of the extrapolated Cayley transform, respectively.

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1. Introduction

We call a non-Hermitian matrix positive definite (semidefinite) if its Hermitian part is positive definite (semidefinite). Let $P \in \mathbb{C}^{n\times n}$ be a non-Hermitian and positive semidefinite matrix, and $\mathbb{R}_+ = \{\alpha \mid \alpha \in \mathbb{R},\ \alpha > 0\}$. Define the mapping $V : \mathbb{C}^{n\times n} \times \mathbb{R}_+ \to \mathbb{C}^{n\times n}$ by

$$V(P,\alpha) = (\alpha I + P)^{-1}(\alpha I - P),$$

where I is the identity matrix. Then we call $V(P,\alpha)$ the *extrapolated Cayley transform* (**ECT**). Note that $V(P) := V(P,1)$ is the Cayley transform. We remark that the original Cayley transform, described by Arthur Cayley in 1846, is a mapping between skew-symmetric matrices and special orthogonal matrices. The Cayley transform and its extrapolated variant appear in many areas of mathematical science, scientific computing and engineering applications such as numerical solutions of symplectic, unitary and isospectral differential systems [26,27], rational preconditioners for subspace iteration methods in matrix eigenvalue computations [56], preconditioning and iterative methods for systems of linear equations [58,13,12,19], modulus-based iteration methods for linear complementarity problems [22,28], discretization of Lie-group equations [53,62,44], unitary space–time modulation for communicating [42,41,45], and micromagnetics [49].

The Euclidean norm of the ECT $V(P,\alpha)$ bounds the asymptotic convergence rates of many matrix splitting iteration methods such as (i) the *alternating direction implicit* (**ADI**) method [58,1,36,61], the *Hermitian and skew-Hermitian splitting* (**HSS**) method [13,10], the *normal and skew-Hermitian splitting* (**NSS**) method [14], the *positive-definite and skew-Hermitian splitting* (**PSS**) method [12], the shift-splitting preconditioning method [18] and the triangular skew-Hermitian splitting method [50,60,17,51] for solving large sparse and non-Hermitian positive-definite systems of linear equations, (ii) the *preconditioned HSS* (**PHSS**) method [15,11], the *accelerated HSS* (**AHSS**) method [9,4], the dimensional split preconditioning method [20] and the *block alternating splitting implicit* (**BASI**) method [7] for solving large sparse saddle-point linear systems, (iii) the modulus method [22,47,57,52], the modified modulus method [28], the extrapolated modulus method [38,40,37] and the modulus-based splitting methods [6] for solving large sparse linear complementarity problems, and (iv) the *alternately linearized implicit* (**ALI**) method [16], the structure-preserving doubling algorithm [35,54,43,23] and the inexact Newton methods based on doubling iteration scheme [32] for computing the minimal nonnegative solutions of large sparse nonsymmetric algebraic Riccati equations; see also [31,15,21,3,8,63,7,2] and the references therein.

To our knowledge, there has not been much discussion about properties and estimates for the spectral radius and the Euclidean norm of the ECT $V(P,\alpha)$; see [48,55,24,12]. According to the spectral radius, however, Hadjidimos and Tzoumas derived an optimal upper bound in [38,39] by making use of the geometrical tools such as Möbius