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# A residual based error estimate for Leja interpolation of matrix functions

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ABSTRACT

Recent applications in science and engineering require a reliable implementation of the action of the matrix exponential and related $\varphi$ functions. For possibly large matrices an approximation up to a certain tolerance needs to be obtained in a robust and efficient way. In this work we consider Leja interpolation for performing this task. Our focus lies on a new a posteriori error estimate for the method. We introduce the notion of a residual based estimate, where the residual is obtained from differential equations defining the $\varphi$ functions. The properties of this new error estimate are investigated and compared to an existing one. Further, a numerical investigation is performed based on test examples originating from spatial discretization of time dependent partial differential equations in two and three space dimensions. The experiments show that this new approach is robust for various types of matrices and applications.



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## 1. Introduction

The computation of matrix functions is of great importance in many fields of science. The subject started as a topic in pure mathematics, but as there are a wide variety of applications in science and engineering, it soon became interesting also for applied mathematics. An introduction to the field of matrix functions can be found in Higham [11]. One area of applications are differential equations. For the solution of differential equations the matrix exponential is an essential tool. In Moler and Van Loan [15] a non-comprehensive but elaborate list of methods computing the matrix exponential is presented. This includes methods like diagonalization and Padé approximation. Both methods are reasonable and (more importantly) feasible for small dimensional matrices only. For large matrices they soon become inefficient. Fortunately, for the solution of differential equations one needs to compute the action of the matrix function on a vector and not the matrix function itself. Krylov subspace methods, see Saad [16,17], were among the first methods considered to solve this task in an efficient way.

The efficient computation of matrix functions acting on a vector is of importance in many different areas of scientific computing. Among others it allows the implementation of exponential integrators which heavily rely on the stable computation of this action. One of the first competitive implementations is described in Hochbruck et al. [12]. Exponential integrators make use of the so-called $\varphi$ functions, entire functions that are closely related to the exponential function. Recent developments in their implementation made exponential integrators an attractive choice for the time integration of large systems of stiff differential equations. In general, the required action of the matrix function is computed up to a specified tolerance. To do so, one needs to rely on stopping criteria derived from an error estimate. One approach for defining an a posteriori error estimate for Krylov subspace methods can be found in Frommer and Simoncini [10].

Within the class of Krylov subspace methods, there are many competitive methods for computing the action of matrix functions. A comparison of various methods can be found in Caliari et al. [5]. One of these methods is the so-called Leja method, i.e. a polynomial interpolation at Leja points, see Caliari et al. [6]. The standard a posteriori estimate used to determine the quality of the approximation is given by the difference of two successive approximations. This estimate relies on the accurate computation of the required divided differences, see Caliari [4]. However, it will decrease even though the solution might stagnate due to rounding errors. In this paper, we propose a new estimate based on a residual equation suggested in Botchev et al. [3]. The residual estimate has the same asymptotic behavior as the interpolation error and indicates stagnation of the approximation. Furthermore, we extend this residual approach to the $\varphi$ functions and point out the corresponding residual equations. The new error estimate is then applied to Leja interpolation and examined with the help of examples resulting from spatial discretizations of time dependent partial differential equations in two and three space dimensions.