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ON SMOOTH LU DECOMPOSITIONS WITH APPLICATIONS TO SOLUTIONS OF NONLINEAR EIGENVALUE PROBLEMS*

Hua Dai
Department of Mathematics, Nanjing University of Aeronautics and Astronautics
Nanjing 210016, China
Email: hdai@nuaa.edu.cn
Zhong-Zhi Bai
LSEC, ICMSEC, Academy of Mathematics and Systems Science, Chinese Academy of Sciences
Beijing 100190, China
Email: bzz@lsec.cc.ac.cn

Abstract

We study the smooth LU decomposition of a given analytic functional λ-matrix $A(\lambda)$ and its block-analogue. Sufficient conditions for the existence of such matrix decompositions are given, some differentiability about certain elements arising from them are proved, and several explicit expressions for derivatives of the specified elements are provided. By using these smooth LU decompositions, we propose two numerical methods for computing multiple nonlinear eigenvalues of $A(\lambda)$, and establish their locally quadratic convergence properties. Several numerical examples are provided to show the feasibility and effectiveness of these new methods.

Mathematics subject classification: 15A18, 15A23, 65F15.
Key words: Matrix-valued function, Smooth LU decomposition, Pivoting, Nonlinear eigenvalue problem, Multiple eigenvalue, Newton method.

1. Introduction

The importance of constant matrix decompositions cannot be overstressed, as they are not only basic methods in matrix computations and analyses, but also applicable tools in other areas beyond mathematics. However, the smooth decompositions of matrices depending on some parameters are by no means less important.

In fact, fundamental theory on decompositions of a matrix-valued function $A(\lambda)$ is given in Kato's book [21], in which one of the strongest results is that $A(\lambda)$ has an analytic spectral decomposition in the case that $A(\lambda)$ is real, analytic and Hermitian. Here, $A(\lambda) = (a_{ij}(\lambda))$ denotes an n-by-n matrix with all elements $a_{ij}(\lambda)$, $i, j = 1, 2, \ldots, n$, being analytic functions with respect to a real or a complex parameter λ; it is called a functional λ-matrix in [20] or a matrix-valued function in [26]; in particular, if $a_{ij}(\lambda)$ are polynomials in λ, then it is called a λ-matrix or a matrix polynomial in [25]. Based on the work in [20,23,34], Li [27,28] developed QR decomposition and its block-analogue for a differentiable matrix-valued function, and gave sufficient conditions for guaranteeing the existence of a differentiable QR decomposition. In [6] the authors showed that a real analytic matrix-valued function admits an analytic singular value decomposition, and Wright further presented a numerical method in [43] for finding a

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smooth singular value decomposition of a matrix solely depending on a single parameter. It is noticed that Gingold and Hsieh [13] used a different approach to show that a real analytic matrix-valued function with only real eigenvalues admits an analytic Schur decomposition. Then, Dieci and Eirola [10] considered smooth QR, smooth Schur, and smooth singular value decompositions as well as their block-analogues, gave sufficient conditions for guaranteeing the existence of such matrix decompositions, and derived differential equations for the involved factors. Recently, Rebaza [33] applied smooth block Schur decompositions of matrix-valued functions to numerical computations of the separatrices in dynamical systems, and analyzed the actual implementations of the correspondingly induced numerical method.

One important application of the above-described smooth matrix decompositions is that they may lead to effective numerical methods for solving *nonlinear eigenvalue problems* (**NEPs**) of the form

$$A(\lambda)x = 0, \tag{1.1}$$

where λ and x, known as the eigenvalue and the eigenvector, respectively, are the variables to be determined. The NEP (1.1), including the typical linear and quadratic eigenvalue problems as special cases, is of great importance in a large number of disciplines of scientific computing and engineering applications such as density functional theory calculations [4], vibration of viscoelastic structures [9], dynamic finite element method [11], photonic band structure calculations [38], vibration of fluid-solid structures [40], and so on.

When $A(\lambda)$ is a matrix polynomial, the NEP (1.1) can be reformulated as a linear eigenvalue problem [24, 31] and, hence, it may be effectively solved by the Jacobi-Davidson method; see, e.g., [19,36]. In general, the NEP (1.1) may be first reformulated as a system of nonlinear equations through either adding a normalization equation $v^*x = 1$ or computing the characteristic polynomial $c(\lambda) := \det(A(\lambda))$, and then solve the so-obtained nonlinear system by utilizing the classical Newton method, see [2, 22, 25, 34], where and in the sequel, $\det(\cdot)$ is used to represent the determinant of the corresponding matrix. Here, the vector v^*, the conjugate transpose of the complex vector v, can be chosen flexibly so that either the nonlinear function may satisfy certain desired property or various iteration methods can be produced. For example, for $v = x$ we can obtain the Rayleigh quotient iteration, see [24, 25, 34].

It was shown in [34] that the Newton method resulted from the first approach is equivalent to the inverse iteration discussed in [39], which converges quadratically under the nondegeneracy condition [37, 38]. However, the inverse iteration requires to solve a linear system with the coefficient matrix $A(\lambda^{(k)})$ at each iteration step k. The Newton method resulted from the second approach has the succinct expression

$$\lambda^{(k+1)} = \lambda^{(k)} - \frac{1}{\operatorname{tr}\left(A(\lambda^{(k)})^{-1}A'(\lambda^{(k)})\right)}, \qquad k = 0, 1, 2, \ldots,$$

where $\operatorname{tr}(\cdot)$ denotes the trace of the corresponding matrix and $A'(\lambda^{(k)})$ the derivative with respect to the variable λ of the matrix-valued function $A(\lambda)$ at $\lambda = \lambda^{(k)}$. For details, we refer to [22, 25]. Once the eigenvalues are available, the eigenvectors can be approximated by the inverse iteration [32, 37]. However, we should mention that the latter approach is less efficient for larger matrices. We refer to [1] for another elegant derivation of a scalar function having the same zeros as $c(\lambda)$ and for several iteration methods.

To overcome the disadvantages of the afore-described Newton-type methods, many authors have presented and analyzed various iteration methods such as the modified inverse iteration [29], the Arnoldi method [41], the rational Krylov subspace method [35], and the Jacobi-