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A generalized Steffensen's method for matrix sign function

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ARTICLE INFO	A B S T R A C T
MSC: 65F60	A direct generalized Steffensen's method is proposed for solving the quadratic matrix equation $F(X) := X^2 - I = 0$. In this way, when the matrix <i>A</i> is nonsingular, we derive a new numerical scheme for finding matrix sign function. The local and global convergence of the proposed generalization is brought up via the concept of basins of attraction. We also report some numerical results of the proposed method, which show its applicability.
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1. Introduction

The matrix sign decomposition [7] is defined for $A \in \mathbb{C}^{n \times n}$ having no pure imaginary eigenvalues as follows

$$A = SN = A(A^2)^{-1/2}(A^2)^{1/2}.$$

Here, S = sign(A) is the matrix sign function, introduced for the first time by Roberts in [12]. We herewith remark that in this work, whenever we write about the computation of a matrix sign function, we mean a square matrix with no eigenvalues on the imaginary axis. This implies that A is nonsingular. Note that functions of matrices play an important role in many applications. If

$$A = T I_A T^{-1} \in \mathbb{C}^{n \times n},\tag{2}$$

is a Jordan canonical form arranged so that

$$J_A = \begin{pmatrix} J_A^{(1)} & 0\\ 0 & J_A^{(2)} \end{pmatrix},\tag{3}$$

where the eigenvalues of $J_A^{(1)} \in \mathbb{C}^{p \times p}$ lie in the open left half-plane and those of $J_A^{(2)} \in \mathbb{C}^{q \times q}$ lie in the open right half-plane, with p + q = n, then

$$S = \operatorname{sign}(A) = T \begin{pmatrix} -l_p & 0 \\ 0 & l_q \end{pmatrix} T^{-1}.$$
(4)

Note that sign(A) is a primary matrix function corresponding to the scalar sign function

$$sign(z) = \begin{cases} 1, & Re(z) > 0, \\ -1, & Re(z) < 0, \end{cases}$$
(5)

which maps *z* to the nearest square root of unity.

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Iteration methods are the most widely used schemes for computing S. Newton's method expressed by

$$X_{k+1} = \frac{1}{2} (X_k + X_k^{-1}), \tag{6}$$

is one of the most reliable methods for S, (see [8,12]). It converges quadratically when

$$X_0 = A.$$
(7)

has been chosen as the initial matrix and is numerically stable.

In this paper, we focus on extending the root-finding Steffensen's method for the matrix sign function *S*. We are mainly concerned with Steffensen's method for finding the solution of the nonlinear matrix equation,

$$F(X) := X^2 - I = 0,$$
(8)

when of course sign(A) is one solution of this equation (see for more details [14,15]).

The remaining sections of this work are organized in what follows. To develop a new method and investigate its convergence characteristics, in Section 2 we give some basic concepts and a direct generalization of Steffensen's method for a special quadratic equation. Following the work [6], we expose a natural classification of iterative methods extracted from Steffensen's family to have global convergence. Properties of the presented matrix iterative family of methods, such as order of convergence, are considered in Section 3. Several numerical examples are given to illustrate the efficiency and performance of the new generalized Steffensen's method in Section 4. A summary of the paper is brought up in Section 5.

2. Generalized Steffensen's method

Starting from a suitable scalar x_0 , the Steffensen's family of method [19] uses the iteration:

$$x_{k+1} = x_k - \frac{f(x_k)}{f[x_k, w_k]}, \quad k = 0, 1, 2, \dots,$$
(9)

wherein $w_k = x_k + \beta f(x_k)$, $f[x_k, w_k]$ is the two-point divided difference, and $\beta \in \mathbb{R} \setminus \{0\}$. It is known that this method has second order of convergence, for every non-zero value of the parameter β provided that an enough close initial approximation for a nonlinear equation is given [10].

The importance of the Steffensen's method is in the fact that it has the same order and computational cost as the Newton's method, but it is free from derivative. This motivated many authors to work on this type of iterative methods [16]. It is remarked that the parameter $\beta \neq 0$ plays an *important* role for the stability of the method (9) as fully discussed in [6]. Thus, in this section we follow the theoretical and practical discussions of [6] so as to generalize (9) for matrix sign.

Now, we apply (9) for solving the following quadratic equation

$$g(x) := x^2 - 1 = 0. \tag{10}$$

Consequently, we obtain a family of quadratically convergent schemes as follows:

$$x_{k+1} = \frac{1 + x_k^2 - \beta x_k + \beta x_k^3}{2x_k - \beta + \beta x_k^2}, \quad k = 0, 1, 2, \dots$$
(11)

Remark 2.1. A function f(A) can be the solution of a matrix equation F(X; A) = 0. And a natural way to compute it is to use iterative root-finding algorithms.

The free parameter β gives a generality to (11). It is mentioned that $\beta = 0$ results in the Newton's iteration (6) and shows that our approach includes this important method as one of its members. However, an important barrier occurred which is non-global convergence of some of the schemes extracted from (11) for the quadratic equation (10) [5].

On the other side, the matrix convergence is governed by the scalar convergence. To be more precise, this is true for the matrix sign function when the scalars are eigenvalues.

Hence, we should find members from (11), at which the derived new methods have global convergence. Toward this goal, we employ the theory of basins of attraction for (11) so as to solve (10) in the square of $[-2, 2] \times [-2, 2]$ of the complex plane, whereas the maximum number iterates are set to 100 and the stopping criterion is $|g(x_k)| \le 10^{-4}$ in our written programmes. We consider the black areas as the points which make the method to diverge and the white points as the exact location of the simple roots of (10), i.e. ± 1 .

The attraction basins are brought forward in Figs. 1–4 for different values of β . In Figs. 1A–4A, the convergence is locally, and therefore convergence of matrix iterations could happen only for very sharp initial matrices X_0 . Accordingly, this put them out of interest. We remark that β has been chosen according to the theoretical discussions of [6].

From Fig. 4B and further investigations based on various smaller values of β , which have not been included in this section, we achieve the point that the convergence of (11) for the quadratic equation (10) is global once $|\beta| \le 0.001$ and $\beta \ne 0$.

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