Fixed Point Iterations for Computing Square Roots and the Matrix Sign Function of Complex Matrices

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Abstract

The purpose of this work has been the development of new set of rational iterations for computing square roots and the matrix sign function of complex matrices. Given any positive integer $r \geq 2$, we presented a systematic way of deriving rth order convergent algorithms for matrix square roots, the matrix sign function, invariant subspaces in different half-planes, and the polar decomposition. We have shown that these iterations are applicable for computing square roots of more general type of matrices than previously reported, such as matrices in which some of its eigenvalues are negative. Also, algorithms for computing square roots and the invariant subspace of a given matrix in any given half-plane are derived.

1 Introduction

The principal square root and the matrix sign functions of complex matrices have several applications in systems and control theory. The principal square root of a positive definite matrix is required in many algorithms in signal processing and control. The matrix sign function can be applied to solve the matrix Lyapunov and Riccati equations and to approximate some matrix-valued functions [1], [2]. It has also been used for block diagonalization of complex matrices [3]. The number of eigenvalues of a matrix with positive and negative real parts can be obtained using the matrix sign function [3], [4]. The matrix sign function was utilized in [4] for eigenvalue separation in different regions in the complex plane. A comprehensive treatment of the matrix sign function and its applications can be found in [1], [3].

There are many techniques in the literature for the computation of the principal square root and the matrix sign function of complex matrices. In [2], the matrix sign algorithm is developed. In [3], Denman et al. developed methods for the computations and possible applications of the matrix sign function. A matrix continued fraction method for computing square roots was presented in [5]. Computational methods for roots of real matrices whose eigenvalues have nonzero real part was developed in [6], where root of real matrices is computed using the sign matrix and a set of projectors. The Newton-Raphson method was applied for computing the pth roots of positive definite matrices [7]. An accelerated algorithm for computing the positive definite square root of a positive definite matrix was presented in [8]. Several variants of Newton's method and their implementations were presented in [9]-[11]. Stable methods for computing square roots was developed in [12], [13]. Theory and algorithms for the matrix sign function were presented in [14]-[17]. Numerically efficient methods for computing the polar decomposition of nonsingular complex matrices can be found in [18]-[23].

Let $A \in \mathcal{C}^{m\times m}$ be a complex matrix, where $\mathcal{C}$ is the field of complex numbers. Then $A = P^{-1}(\Lambda + N)P$, for some nonsingular matrix P, $\Lambda = \text{diag}(\lambda_1, \cdots, \lambda_m)$ and N is nilpotent matrix that commutes with D. Define the sign of A by $S_2(A) = \text{sign}(A) = P\text{diag}(\text{sign}(\lambda_1), \cdots, \text{sign}(\lambda_m))P^{-1}$, where for any $z = x + iy \in \mathcal{C}$ with $x \neq 0$,

$$\text{sign}(z) = \text{sign}(x + iy) = \text{sgn}(x) \tag{1a}$$

and

$$\text{sgn}(x) = \begin{cases} 1 & \text{if } x > 0, \\ -1 & \text{if } x < 0. \end{cases} \tag{1b}$$

The principal square root of the complex matrix A is defined to be any matrix $B \in \mathcal{C}^{m\times m}$ such that $B^2 = A$ and for every $\gamma_r \in \sigma(B)$, $\sigma(A)$ denotes the set of eigenvalues of A, we have $\gamma_r = |\gamma_r|e^{i\theta_r}$, where $\theta_r \in (\frac{-\pi}{2}, \frac{\pi}{2})$, for $r = 1, \cdots, m$ and i is the complex number $\sqrt{-1}$. From the above introduction we observe that the matrix sign function is a square root of the identity matrix which commutes with A. Specifically, $S_2(A)^2 = I_m$, and $AS_2(A) = S_2(A)A$ has all of its eigenvalues in the sector $\frac{-\pi}{2} < \theta < \frac{\pi}{2}$, i.e., $S_2(A)A$ has all its eigenvalues in the right half plane. These two conditions can be viewed as a characterization of the matrix sign function.

The matrix sign function provides an elegant way of splitting C^2 into two complementary subspaces; the "table"and "unstable" invariant subspaces of some matrix A, without actually computing any eigenvalues. The matrix $S_2(A)$ is diagonalizable and has the same stable and unstable invariant subspaces as A; its eigenvalues are -1 and +1, corresponding to eigenvalues of A with negative and positive real part, respectively. The columns of $S_2(A) - I_m$ and $S_2(A) + I_m$ span the invariant subspaces associated with the left and right half plane eigenvalues of A, respectively. Some good references on the matrix sign function and/or its application to solving the algebraic Riccati equation are Roberts [2], Byers [15], Byers, He and Mehrmann [16], Gander [20] and Kenny, Laub [23].

2 Rational Fixed Point Functions

The computation of square roots of complex matrices has been extensively investigated in the literature. The Newton-Raphson method was used in [9] for computing the principal square root of a complex matrix. The fixed point function for the standard Newton's method for solving the equation $F(Y) = 0$ takes the form $\Phi(Y) = Y - F'(Y)^{-1}F(Y)$. A modified version of Newton's method which is useful in computing multiple zeros of F has the fixed point function $\Phi(Y) = Y - \{F'^2(Y) - F(Y)F''(Y)\}^{-1}F'(Y)F(Y)$. Newton's method is known to have quadratic convergence in a neighborhood of a simple zero of F. In [10] a second order iteration for computing square roots of matrices having eigenvalues with nonzero real parts is developed. Halley's method for solving $F(Y) = 0$ is known to be cubically convergent and has the fixed point function $\Phi(Y) = Y - \{F'^2(Y) - \frac{1}{2}F(Y)F''(Y)\}^{-1}F'(Y)F(Y)$. In this section, higher order fixed point iterations which generalize Newton's and Halley's methods for computing a square root of a complex matrix with possibly some negative eigenvalues are developed. We should note that the main feature of these methods is that the square root which these iterations converge to is determined by the initial condition. In what follows, we consider fixed point functions of rational form of two polynomials $C_r(Y, A)$ and $D_r(Y, A)$ which are defined for each integer $r \geq 1$ as follow:

$$C_r(Y, A) = \sum_{l=0}^{\lfloor \frac{r}{2} \rfloor} \binom{r}{2l} Y^{r-2l} A^l, \tag{2a}$$

and

$$D_r(Y, A) = \sum_{l=0}^{\lfloor \frac{r}{2} \rfloor} \binom{r}{2l+1} Y^{r-2l-1} A^l, \tag{2b}$$

where $\lfloor \frac{r}{2} \rfloor$ denotes the largest integer less than or equal to $\frac{r}{2}$. For each positive integer r we define

$$\Phi_r(Y, A) = D_r(Y, A)^{-1} C_r(Y, A). \tag{2c}$$

It will be shown in Section 3 that Φ_r is a fixed point iteration of order r for the equation $X^2 - A = 0$.

When Y is a scalar, the functions C_r and D_r have some interesting properties as described in the following proposition. Some of these properties also hold when Y is a square matrix.

Proposition 1. *Let A be a nonsingular matrix and let X be a square root of A. For each positive integer $r \geq 1$ let C_r and D_r be as defined in (2) and let Y be any matrix that commutes with X. Then*

- *(i) C_r and D_r satisfy the identities $C_r(Y, A) + D_r(Y, A)X = (Y + X)^r$ and $C_r(Y, A) - D_r(Y, A)X = (Y - X)^r$.*
- *(ii) $C_r(Y, A) = \frac{1}{2}\{(Y + X)^r + (Y - X)^r\}$ and $D_r(Y, A) = \frac{1}{2}\{(Y + X)^r - (Y - X)^r\}X^{-1}$.*
- *(iii) In the scalar case, the polynomials C_r and D_r are relatively prime.*
- *(iv) Let $C_1(Y, A) = Y$ and $D_1(Y, A) = I_m$, then C_r and D_r, for $r \geq 2$, can recursively be generated as follows*

$$C_r(Y, A) = Y C_{r-1}(Y, A) + D_{r-1}(Y, A)A,$$

and

$$D_r(Y, A) = Y D_{r-1}(Y, A) + C_{r-1}(Y, A).$$

- *(v) In the scalar case, the polynomials C_r and C_{r+1} are relatively prime.*
- *(vi) C_r is even when r is even and is odd when r is odd.*
- *(vii) D_r is even when r is odd and is odd when r is even.*
- *(viii) In the scalar case, $\frac{d}{dY}C_r(Y, A) = rC_{r-1}(Y, A)$, and $\frac{d^l}{dY^l}C_r(Y, A) = r(r-1)\cdots(r-l+1)C_{r-l}(Y, A)$, for $l \geq 1$.*
- *(ix) $\frac{d}{dY}D_r(Y, A) = rD_{r-1}(Y, A)$, and $\frac{d^l}{dY^l}D_r(Y, A) = r(r-1)\cdots(r-l+1)D_{r-l}(Y, A)$, for $l \geq 1$.*

3 Recursive Derivation of $\Phi_r(Y)$

The function Φ_r defined in (2c) can be generated recursively as in the next result.

Proposition 2. *Let A be nonsingular matrix and let X be a square root of A. Let $\Phi_1(Y) = Y$, then for $r > 1$, Φ_r can recursively be generated as follows*

$$\Phi_r(Y, A) = \{\Phi_{r-1}(Y, A) + Y\}^{-1}\{Y\Phi_{r-1}(Y, A) + A\}, \tag{3a}$$

and for $1 \leq l < r$,

$$\Phi_r(Y, A) = \{\Phi_{r-l}(Y, A) + \Phi_l(Y, A)\}^{-1}\{\Phi_l(Y, A)\Phi_{r-l}(Y, A) + A\}. \tag{3b}$$

Proof. From the definitions of $\Phi_r(Y, A)$ and Proposition 1, we have

$$\Phi_r(Y, A) = D_r(Y, A)^{-1}C_r(Y, A)$$
$$= \{YD_{r-1}(Y, A) + C_{r-1}(Y, A)A\}^{-1}\{YC_{r-1}(Y, A)$$
$$+ D_{r-1}(Y, A)A\} = \{\Phi_{r-1}(Y, A) + Y\}^{-1}\{Y\Phi_{r-1}(Y, A) + A\}.$$

Part (3b) can be established similarly.

Q.E.D.

In the next theorem it will be shown that, for each integer $r \geq 1$, every square root of A is a fixed point of the function $\Phi_r(Y, A)$.

Theorem 3. *Let A be a nonsingular diagonalizable matrix and let r be a positive integer such that $r \geq 2$ and let C_r and D_r be as defined in (2). Assume that X is a square root of A and that Y commutes with A. Then the function $\Phi_r : \mathcal{C}^{m\times m} \to \mathcal{C}^{m\times m}$ given by $\Phi_r(Y, A) = D_r(Y, A)^{-1}C_r(Y, A)$ defines an rth order fixed point function, i.e., $\Phi_r(X, A) = X$ and $\frac{d^l}{dY^l}\Phi_r(X, A) = 0$, for $l = 1, 2, \cdots, r-1$. Moreover,*

$$\frac{d}{dY}\Phi_r(Y, A) = rD_r(Y, A)^{-1}(Y^2 - A)^{r-1}, \text{ holds for the scalar case}$$

and

$$\{\Phi_r(Y, A) + X\}^{-1}(\Phi_r(Y, A) - X) = \{(Y + X)^{-1}(Y - X)\}^r. \tag{4}$$

Moreover, Φ_r can uniquely be determined from the error formula (4).

4 Choice of Initial Conditions and Convergence Analysis

We have shown that Φ_r is a fixed point iteration of order r for the equation $X^2 - I_m = 0$. To compute the fixed points of Φ_r an initial matrix is required. The main conditions that this initial matrix X_0 must satisfy are that it commutes with A and is nonsingular. The importance of the choice of X_0 is that X_0 determines which particular square root of A is a fixed point of Φ_r. The simplest choice of such an X_0 is any polynomial of A. In this section, the convergence of the iteration $X_{k+1} = \Phi_r(X_k, A)$, where $X_0 \in \mathcal{C}^{m\times m}$ is a nonsingular matrix such that $AX_0 = X_0A$ will be analyzed. Let $r \geq 2$ be a fixed integer then the basic iteration can be described as follows:

$$\begin{aligned} &\text{Given } X_0 \text{ with } X_0A = AX_0, \\ &X_{k+1} = D_r(X_k, A)^{-1}C_r(X_k, A) = \Phi_r(X_k, A). \end{aligned} \tag{5a}$$

The analogue of (5a) for computing the matrix sign function can be obtained if the roles of X_0 and A are interchanged. This means that $X_0 = A$ and $A = I_m$, in which case one can show that the iterations in (5b) converge to the matrix sign function of A:

$$\begin{aligned} &\text{Given } X_0 = A, \\ &C_r(X_k, I_m) = \sum_{l=0}^{\lfloor \frac{r}{2} \rfloor} \binom{r}{2l} X_k^{r-2l}, \\ &D_r(X_k, I_m) = \sum_{l=0}^{\lfloor \frac{r}{2} \rfloor} \binom{r}{2l+1} X_k^{r-2l-1}, \\ &X_{k+1} = D_r(X_k, I_m)^{-1}C_r(X_k, I_m) = \Phi_r(X_k, I_m). \end{aligned} \tag{5b}$$

The convergence properties of this iteration is dependent on the initial matrix X_0 and r.

Remark: There are other ways to generate Φ_r. For any two rational functions $P(z)$ and $Q(z)$, if $\frac{P(z)-Q(z)}{P(z)+Q(z)} = (\frac{z-1}{z+1})^r f(z)$ for some rational function f such that $f(-1) \neq 0$, then a fixed point function for computing the matrix sign function can be obtained as

$$\Phi_r(z) = \frac{(z-1)^r f(z) + (z+1)^r}{(z+1)^r - (z-1)^r f(z)}.$$

The conditions that guarantee such formula are $P(1) = Q(1)$, $P(1) = -Q(1)$, and

$$P^{(i)}(1) = Q^{(i)}(1), \quad \textit{and } P^{(i)}(-1) = -Q^{(i)}(-1)$$

for $i = 1, \cdots, r-1$. Then $\Phi_r(z)$ satisfies

$$\frac{\Phi_r(z) - 1}{\Phi_r(z) + 1} = (\frac{z-1}{z+1})^r f(z).$$

In the literature, the choice $X_0 = aI_m$, $0 \leq a \in \mathcal{R}$ is often used [8]-[9]. With this choice, Iteration (5a) converges only if the matrix A has no negative eigenvalues and Iteration (5b) converges if A has no pure imaginary eigenvalues. Thus this initial guess is usful only if the principal square root is of interest. It turns out (see Proposition 4) that this limitation can partially be overcome by using initial matrices of the form $X_0 = bI_m$, $b \in \mathcal{C}$ with nonzero imaginary part. Other choices of X_0 such as the matrix sign function of A and in fact any nonsingular matrix which commutes with A will also be considered. The effect of the eigenstructure of X_0 on the convergence of (5a) and (5b) is described in the next result.

Proposition 4. *Let X and X_0 be commutative nonsingular matrices and let P be a nonsingular matrix such that $P^{-1}X_0P$ and $P^{-1}XP$ are in canonical Jordan form. Assume that $\lambda_j(X_0) = u_j + iv_j$ and $\lambda_j(X) = x_j + iy_j$, where $u_j, v_j, x_j, y_j \in \mathcal{R}$, $j = 1, \cdots, m$. Then*

(i) $|\lambda_j(X_0) - \lambda_j(X)| < |\lambda_j(X_0) + \lambda_j(X)|$ *if and only if* $u_jx_j + v_jy_j > 0$ *for* $j = 1, \cdots, m$.

(ii) If $X_0 \in \mathcal{C}^{m\times m}$ is nonsingular with real eigenvalues, and no eigenvalue of X lies on the imaginary axis, then $\text{sign}(X) = \text{sign}(X_0)$, *if and only if* $|\lambda_j(X_0) - \lambda_j(X)| < |\lambda_j(X_0) + \lambda_j(X)|$, *for* $j = 1, 2, \cdots, m$.

(iii) if $X_0 = A$ and X is a square root of A with $P^{-1}XP =$ $\text{diag}(x_1+iy_1, \cdots, x_m+iy_m)$, *then* $|\lambda_j(A-X)| < |\lambda_j(A+X)|$, *if and only if* $x_j > 0, j = 1, 2, \cdots, m$.

The significance of Proposition 4 is that it makes it possible to develop algorithms for computing square roots of matrices which have negative eigenvalues. Combining the result of Theorem 3 and Proposition 4, we obtain the following result which provides an rth order algorithm for computing the square root of any nonsingular matrix.

Theorem 5. *Let A be a nonsingular matrix and let r be a positive integer such that $r \geq 2$. Let X be a square root of A and let X_0 be a nonsingular matrix such that $X_0A = AX_0$ and $|\lambda_j(X_0) - \lambda_j(X)| < |\lambda_j(X_0) + \lambda_j(X)|$ for $j = 1, 2, \cdots, m$. Then the sequence $\{X_k\}_{k=1}^{\infty}$ generated by Iteration (5a) converges of order r to X, with the following error formulas*

$$(X_{k+1} + X)^{-1}(X_{k+1} - X) = \{(X_k + X)^{-1}(X_k - X)\}^r, \tag{6a}$$

or equivalently

$$(X_k + X)^{-1}(X_k - X) = \{(X_0 + X)^{-1}(X_0 - X)\}^{r^k}. \tag{6b}$$

Hence the sequence X_k converges to X, where X is the unique square root of A for which $u_jx_j + v_jy_j > 0$, where $x_j = Re(\lambda_j(X))$, $y_j = Im(\lambda_j(X))$, $u_j = Re(\lambda_j(X_0))$, $v_j = Im(\lambda_j(X))$. Specifically, depending on the initial matrix X_0, the sequence $\{X_k\}_{k=1}^{\infty}$ generated by Iteration (5a) converges as in the following cases:

(1) Assume that A has no negative eigenvalue and let $X_0 = (a + ib)I_m$, $a, b \in \mathcal{R}$. Then

- *(i) if $a > 0$, the sequence X_k is rth order convergent to X, where X is the unique square root of A for which every eigenvalue has positive real part.*
- *(ii) If $a < 0$, then the sequence X_k converges to X, where X is the unique square root of A for which every eigenvalue has negative real part.*

(2) Let $X_0 = (a + ib)I_m$, $a > 0, b > 0$. If a is sufficiently large such that $ax_j + by_j > 0$ for $j = 1, \cdots, m$, then the sequence X_k converges to X, where X is the unique square root of A for which every eigenvalue with nonzero real part has same sign as a and such that if for some $j = 1, 2, \cdots, m$, $Re(\lambda_j(X)) = 0$, then $Im(\lambda_j(X))$ has same sign as b.

(3) Assume that A has some negative eigenvalues and that $X_0 = \alpha A + \beta$, where $\alpha = \alpha_1 + i\alpha_2$ and $\beta = \beta_1 + i\beta_2$, with $\alpha_j, \beta_j \in \mathcal{R}$ for $j = 1, 2$. Then the sequence $X_k = \Phi_r(X_k, A)$ converges to X, where X is the unique square root of A for which the inequality

$$(\alpha_1 x_j - \alpha_2 y_j)(x_j^2 + y_j^2) + \beta_1 x_j + \beta_2 y_j > 0, \quad (7)$$

holds for every eigenvalue $x_j + iy_j$ of X.

Proof. The proof follows from simple manipulation of complex numbers.

Q.E.D.

In Theorem 3 if $r = 2$, then the quadratically convergent Newton's algorithm is obtained as shown next.

Corollary 6. *Let A be an $m \times m$ nonsingular complex matrix. Given X_0 and define the following sequence*

$$X_{k+1} = \frac{1}{2}\{X_k + X_k^{-1} A\}. \quad (8)$$

(i) if none of A's eigenvalues is negative real number, and X_0 is a positive definite matrix which commutes with A, then the iterates $\{X_k\}$ converges quadratically to the principal square root X, a square root of A for which every eigenvalue has positive real part.

(ii) if none of A's eigenvalues is negative real number, and if X_0 is a negative definite matrix which commutes with A, then X_k converges quadratically to X, a square root of A for which every eigenvalue has negative real part.

(iii) Let $X_0 = (a + ib)I_m$ such that $a + ib \neq 0$. Then X_k converges quadratically to X, a square root of A for which every eigenvalue $x_j + iy_j$ satisfies $ax_j + by_j > 0$ for $j = 1, \cdots, m$. In particular, if $x_j = 0$ for some j and $b \neq 0$, then X_k converges to X such that for any eigenvalue of X having zero real part its imaginary part has the same sign as b.

The significance of this generalization is that a can be chosen to be any nonzero complex number. As indicated in the last result, this is particularly necessary for computing square roots of matrices having negative eigenvalues or computing sign functions for matrices having eigenvalues on the imaginary axis where the standard matrix sign function is not defined.

5 Computations and Applications to Matrix Decompositions

5.1 Computing Square Roots and Projections in Half Planes

Square roots whose eigenvalues lie in one side of a half plane can be computed by appropriately choosing the initial condition X_0. One way to establish that is by applying the iteration $X_{k+1} = \Phi_r(X_k)$ to compute the square root of $\alpha^2 A$ where α is any nonzero complex number lying on the boundary of the half plane. The convergence of the resulting iteration can be analyzed using the error formula

$$(X_{k+1} + \alpha X)^{-1}(X_{k+1} - \alpha X) = \{(X_k + \alpha X)^{-1}(X_k - \alpha X)\}^r, \quad (9a)$$

or equivalently

$$(X_k + \alpha X)^{-1}(X_k - \alpha X) = \{(X_0 + \alpha X)^{-1}(X_0 - \alpha X)\}^{r^k}. \quad (9b)$$

This means that X_k converges to αX, where X is a square root of A for which $||X_0 - \alpha X|| < ||X_0 + \alpha X||$. Hence if $\alpha = -1$ and A has no pure imaginary eigenvalues, then the iteration $X_{k+1} = \Phi_r(X_k, A)$, $X_0 = A$ will converge to iX where X is a square root of A whose eigenvalues have negative imaginary part.

It is interesting to note that several useful variations of Newton's method for computing invariant subspaces and square roots of a matrix in different half-planes can be obtained. For example, the iteration

$$X_0 = A, \quad X_{k+1} = \frac{1}{2}\{X_k - X_k^{-1} A\}, \quad (10a)$$

converges to iX where X is a square root of A whose eigenvalues are in the upper half plane. Similarly, the iteration

$$X_0 = A, \quad X_{k+1} = \frac{1}{2}\{X_k - X_k^{-1}\}, \quad (10b)$$

converges to a matrix S satisfying $S^2 = I_m$, $SA = AS$, and all eigenvalues of SA are in the upper half plane.

Generaly, this observation can be utilized to find invariant subspaces of different sectors of the complex plane. For example the iteration

$$X_0 = \alpha A, \alpha \neq 0, \quad X_{k+1} = \frac{1}{2}\{X_k + X_k^{-1}\}, \quad (10c)$$

converges to a matrix S satisfying $S^2 = I_m$, $SA = AS$, and all eigenvalues of SA are all in one side of the half-plane defined by the line passing through origin and α. Note that if A has no eigenvalues on the boundary of the half plane, then the number of positive and negative eigenvalues of S represents the number of eigenvalues of A in the upper and lower half planes, respectively.

5.2 Computation of the Sign Decomposition

The matrix sign decomposition can be used to uniquely decompose the matrix A as $A = NS_2(A)$, where N is a matrix whose eigenvalues in the right half plane and S_2 is involution, i.e., $S_2^2 = I_m$. The following identity links the matrix sign function and the principal square root [13]:

$$S_2(\begin{bmatrix} 0 & I_m \\ A & 0 \end{bmatrix}) = \begin{bmatrix} 0 & A^{\frac{-1}{2}} \\ A^{\frac{1}{2}} & 0 \end{bmatrix}. \quad (11a)$$

where $A^{\frac{1}{2}}$ is the principal square root of A. To compute N, iterations can be developed using the identity

$$S_2(\begin{bmatrix} 0 & I_m \\ A^2 & 0 \end{bmatrix}) = \begin{bmatrix} 0 & A^{-1}S_2(A) \\ AS_2(A) & 0 \end{bmatrix} = \begin{bmatrix} 0 & N^{-1} \\ N & 0 \end{bmatrix}. \quad (11b)$$

This holds true since $\begin{bmatrix} 0 & A^{-1}S_2(A) \\ AS_2(A) & 0 \end{bmatrix}^2 = I_{2m}$, and

$$\begin{bmatrix} 0 & I_m \\ A^2 & 0 \end{bmatrix} \begin{bmatrix} 0 & A^{-1}S_2(A) \\ AS_2(A) & 0 \end{bmatrix} = \begin{bmatrix} AS_2(A) & 0 \\ 0 & AS_2(A) \end{bmatrix} \times \begin{bmatrix} 0 & I_m \\ A^2 & 0 \end{bmatrix} = \begin{bmatrix} N & 0 \\ 0 & N \end{bmatrix}, \quad (12)$$

which has all its eigenvalues in the right half plane.

5.3 The Equation $XBX = A$

The ideas of the previous section can be utilized to solve the quadratic matrix equation

$$XBX = A, \tag{13}$$

where A and B are nonsingular matrices. If none of the eigenvalues of AB are negative, then $S_2(\begin{bmatrix} 0 & A \\ B & 0 \end{bmatrix})$ is defined. From the Newton iteration of the matrix sign function it follows that $S_2(\begin{bmatrix} 0 & A \\ B & 0 \end{bmatrix})$ has the form

$$S_2(\begin{bmatrix} 0 & A \\ B & 0 \end{bmatrix}) = \begin{bmatrix} 0 & C \\ C^{-1} & 0 \end{bmatrix}.$$

for some nonsingular matrix C. Clearly, C is a solution of (13).

5.4 A Power Method For Computing the Matrix Sign Function

Proposition 7. *Let A and S be $m \times m$ nonsingular matrices such that $S^2 = I_m$ and $SA = AS$. Then for any $\alpha > 0$*

$$\begin{bmatrix} A & \alpha I_m \\ \alpha I_m & A \end{bmatrix} = \begin{bmatrix} I_m & I_m \\ S & -S \end{bmatrix} \begin{bmatrix} A + \alpha S & 0_m \\ 0_m & A - \alpha S \end{bmatrix} \begin{bmatrix} I_m & I_m \\ S & -S \end{bmatrix}^{-1}. \tag{14}$$

Therefore, for any integer k

$$\begin{bmatrix} A & \alpha I_m \\ \alpha I_m & A \end{bmatrix}^k = \begin{bmatrix} I_m & I_m \\ S & -S \end{bmatrix} \begin{bmatrix} (A + \alpha S)^k & 0_p \\ 0_p & (A - \alpha S)^k \end{bmatrix} \begin{bmatrix} \frac{1}{2} I_m & \frac{1}{2} S \\ \frac{1}{2} I_m & -\frac{1}{2} S \end{bmatrix}$$
$$= \begin{bmatrix} \frac{1}{2}(A + \alpha S)^k + \frac{1}{2}(A - \alpha S)^k & \frac{S}{2}(A + \alpha S)^k - \frac{S}{2}(A - \alpha S)^k \\ \frac{S}{2}(A + \alpha S)^k - \frac{S}{2}(A - \alpha S)^k & \frac{1}{2}(A + \alpha S)^k + \frac{1}{2}(A - \alpha S)^k \end{bmatrix}.$$

Consequently, $\lim_{k \to \infty} H_2(k)^{-1} H_1(k)$ converges to a matrix S satisfying $S^2 = I_m$ and the eigenvalues of A and αS have the same sign distribution.

Proof: Since the eigenvalues of S are ± 1, it follows that $|\lambda(A + \alpha S)| > |\lambda(A - \alpha S)|$ if and only if $\lambda(A)$ and $\lambda(\alpha S)$ have the same sign.

Q.E.D.

It can be shown by induction that if

$$H^k = \begin{bmatrix} A & \alpha I_m \\ \alpha I_m & A \end{bmatrix}^k = \begin{bmatrix} H_1(k) & H_2(k) \\ H_2(k) & H_1(k) \end{bmatrix},$$

then $H_1(k) = \sum_{r=0}^{k} \binom{k}{r} \alpha^r A^{k-r}$ and $H_2(k) = \sum_{r=1}^{k} \binom{k}{2r-1} \alpha^r A^{k-r}$. Therefore $S_2(A)$ can be approximated as $S_2(A) = \lim_{k \to \infty} H_2(k)^{-1} H_1(k)$ provided $\alpha > 0$. A squaring method can be developed for generating $H, H^2, H^4, \cdots, H^{2^p}$ for sufficiently large p. This would significantly reduce the computational load of the algorithm. The number α can be chosen to stabilize the convergence by choosing $\alpha = \frac{1}{||A||}$ to avoid over- and/or under-flow.

5.5 Computation of the Polar Decomposition

The polar decomposition is a useful tool in many applications. For example, in situations where it is desirable problems of the form

$$\text{minimize}_Q \ ||A - BQ||_F$$

over unitary matrices, where A and B are known matrices and $||X||_F$ denotes the Frobenius norm of X. It can be shown that the solution matrix Q is the polar factor of B^*A. The techniques of this research plan will be employed to compute the polar decomposition of any matrix. To establish this objective, let A be an $m \times m$ complex matrix, then A can uniquely be decomposed as $A = UH$, where U is unitary and H is positive semidefinite. We will use the following identity

$$S_2(\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}) = \begin{bmatrix} 0 & U \\ U^* & 0 \end{bmatrix}, \tag{15}$$

to develop linearly convergent method for U. This can be seen from the relations $AU^* = UA^*$, and $A^*U = U^*A$ which indicate that both are similar to H. Since H is positive definite, all its eigenvalues are in the right half plane. Analogous relations describing the relation between the matrix sign function and the polar decomposition are as follow:

$$S_2(\begin{bmatrix} 0 & I_m \\ AA^* & 0 \end{bmatrix}) = \begin{bmatrix} 0 & UH^{-1}U^* \\ UHU^* & 0 \end{bmatrix}, \tag{16a}$$

and

$$S_2(\begin{bmatrix} 0 & I_m \\ A^*A & 0 \end{bmatrix}) = \begin{bmatrix} 0 & H^{-1} \\ H & 0 \end{bmatrix}. \tag{16b}$$

These two relations will be utilized to compute the factors U and H of the polar decomposition of A.

Next, we present a block decomposition of a matrix which could be useful in the derivation of fast algorithms for computing the polar factors of a matrix.

Theorem 8. *Let A be nonsingular matrix of size m such that $A = UH$, where $U^*U = I_m$, and H is positive definite, then for any complex number α the following identity holds*

$$\begin{bmatrix} \alpha I_m & A^* \\ A & \alpha I_m \end{bmatrix} = \begin{bmatrix} I_m & I_m \\ U & -U \end{bmatrix} \begin{bmatrix} \alpha I_m + H & 0 \\ 0 & \alpha I_m - H \end{bmatrix} \begin{bmatrix} I_m & I_m \\ U & -U \end{bmatrix}^{-1}. \tag{17a}$$

Therefore, if we assume that

$$\begin{bmatrix} \alpha I_m & A \\ A^* & \alpha I_m \end{bmatrix}^k = \begin{bmatrix} H_1(k) & H_2(k) \\ H_2^*(k) & H_3(k) \end{bmatrix}, \tag{17b}$$

then

$$\begin{bmatrix} \alpha I_m & A \\ A^* & \alpha I_m \end{bmatrix}^k = \begin{bmatrix} I_m & I_m \\ U & -U \end{bmatrix} \begin{bmatrix} (\alpha I_m + H)^k & 0 \\ 0 & (\alpha I_m - H)^k \end{bmatrix}$$
$$\times \begin{bmatrix} \frac{1}{2} I_m & \frac{1}{2} U^* \\ \frac{1}{2} I_m & \frac{-1}{2} U^* \end{bmatrix} =$$
$$\begin{bmatrix} \frac{1}{2}\{(\alpha I_m + H)^k + (\alpha I_m - H)^k\} & \frac{1}{2}\{(\alpha I_m + H)^k - (\alpha I_m - H)^k\} U^* \\ \frac{1}{2} U \{(\alpha I_m + H)^k - (\alpha I_m - H)^k\} & \frac{1}{2} U \{(\alpha I_m + H)^k + (\alpha I_m - H)^k\} U^* \end{bmatrix}, \tag{18}$$

then

$$
\begin{aligned}
&H_1(k)^{-1}H_2(k) \to U^*, \;\; H_2^*(k)H_1(k)^{-1} \to U, \\
&H_3(k)H_2^*(k)^{-1} \to U, \\
&H_1(k)^{-1}H_1(k+1) \to \alpha I_m + H, \\
&H_3(k)^{-1}H_3(k+1) \to \alpha I_m + H.
\end{aligned} \tag{19}
$$

Proof: The proof follows directly from the fact that since H is positive definite, then $\lambda(\alpha I_m + H) > \lambda(\alpha I_m - H)$ for any positive value α.

Q.E.D.

If (19) is implemented directly, over- or under-flow will occur when k is large. One can utilize a squaring method like the one suggested in Section 5.4.

6 Conclusion

In this paper, rational fixed point iterations for computing square roots and the matrix sign function of complex matrices are developed and their convergence properties are thoroughly analyzed. Additionally, new methods for computing invariant subspaces in any given half-plane have been developed. The proposed methods are derived by computing certain matrices that commute with a given matrix. The relationship between the matrix sign function, the polar decomposition, and matrix square roots is being exploited to design new approaches for computing, matrix square roots, the matrix sign and polar decompositions. The matrix S defined in Sections 2 and 4 can also be used for block diagonalization of a matrix A. For example if $\frac{I_m+S}{2} = QR$ is the a QR factorization, then Q^*AQ is block diagonal. This issue in addition to rigorous numerical stability of the algorithms stated in this paper will be dealt with in a forthcoming paper. Simulations and numerical evaluation of some of the algorithms will also be established.

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