On the Computation of Matrix Functions for Square Matrices Having Mixed Eigenvalues Using Numerical Hybrid Method

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Abstract: In this paper, a hybrid numerical method for computing matrix functions of square matrices having mixed (distinct real and pure complex) eigenvalues is presented. The suggested technique is first stated and is then proved to be well defined through different stages. The theoretical analysis of the proposal method is then discussed. Some numerical examples are presented to validate the applicability and the accuracy of the obtained analytical results.

Keywords: Matrix functions; Matrix polynomial; Newton divided differences; Square root of matrix; Polar coordinate; Mixed eigenvalues; Mixed interpolation.

1 Introduction

The extension of the concept of a function of a complex variable to matrix functions has attracted the attention of a number of mathematicians since 1883; see the references [5, 6, 9, 11]. It seems that almost every mathematician who became intrigued by the idea proceeded to give his own definition of a matrix function, with little or no attention to conceptions with earlier definitions. As a result there have been distinct definitions of a matrix functions by Sylvester, Fantappie’s, power series definition and M. Dehghan and M. Hajarían (for more details [2, 3]).

There are many methods and techniques for computing matrix functions \( f(A) \) of \( n \)-by-\( n \) matrix \( A \). The majority research dealing with matrix functions contain mainly results of square matrices having real eigenvalues only. Such matrix functions have numerous uses in different applications [6, 9, 11]. Numerical methods for computing matrix functions of square matrices having real eigenvalues had developed rapidly in the past three decades [6]-[11]. They have been applied successfully to numerical simulations in many fields [9]. A large number of papers have presented several methods for computing matrix functions \( f(A) \) (see, Coleman [1]), Van Loan [13], Dehghan and Hajarían [2, 3]). These methods concentrate on matrices having real eigenvalues only.

In this paper, we will discuss computing matrix functions for square matrices having mixed (real distinct and pure complex) eigenvalues. This paper is organized as follows. In section 2, we give some important definitions for computing matrix function \( f(A) \) of square matrices having real (distinct or repeated) eigenvalues. In section 3, we give our new technique for computing \( f(A) \) for square matrices having mixed eigenvalues and we state a new theorem to show and prove that the new definition is well defined by some functions \( G(z) \) and \( H(z) \). In section 4, we illustrate the applicability and the accuracy of our technique by giving several different numerical examples. Finally a brief conclusion ends this paper.

2 Preliminaries

In this section, we introduce some needed definitions and theorems which will be used to implement our new approach. The following definitions are the most generally useful ones:

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(I) Sylvester definition for matrix function [2]

Sylvester, in 1883, proposed the following definition of a matrix function corresponding to the scalar function \( f(z) \) as:

\[
f(A) = \sum_{j=0}^{n} \prod_{i \neq j} \frac{A - \lambda_i I}{\lambda_j} f(\lambda_j)
\]  

(2.1)

where \( A \in \mathbb{C}^{n+1 \times n+1} \) is a square matrix with distinct characteristic roots \( \lambda_0, \lambda_1, \ldots, \lambda_n \) (real). This definition is a direct extension of the Lagrange interpolation formula for a polynomial \( p(z) \) of degree \( n \), which is applicable only when \( A \) has distinct real roots.

(II) Power series definition for matrix function [2]

E. Weyer, in 1887, appears to be the first one who gave a convergence criterion for a matrix power series. The power series definition is a natural extension of polynomial functions of a matrix. Let \( f(z) \) be analytic function at \( z = z_0 \) and

\[
f(z) = f(z_0) + \frac{f'(z_0)}{1!}(z - z_0) + \cdots + \frac{f^{(k)}(z_0)}{k!}(z - z_0)^k + \cdots
\]

(2.2)

Then one can define the corresponding matrix function:

\[
f(A) = f(z_0) I + \frac{f'(z_0)}{1!}(A - z_0 I) + \cdots + \frac{f^{(k)}(z_0)}{k!}(A - z_0 I)^k + \cdots
\]

(2.3)

provided the series converges.

(III) Fantappie’s Definition for Matrix Function [12]

The eigenvalue method (for example, Goulb and Van Loan, [6]) is an accurate way to compute \( e^A \). However, the speed is generally unacceptable for many applications where fast approximation techniques are desired. Rather than the exact eigenvalue decomposition method, we consider the Padé approximation to the scalar function \( e^z \), is defined by:

\[
e^z \approx R_{pq}(z) = D_{pq}(z)^{-1} N_{pq}(z),
\]

(2.4)

where

\[
N_{pq} = \sum_{k=0}^{p} \frac{(p + q - k)!p!}{(p + q)!k!(p - k)!}(z)^k
\]

(2.5)

and

\[
D_{pq} = \sum_{k=0}^{q} \frac{(p + q - k)!q!}{(p + q)!k!(q - k)!}(-z)^k,
\]

(2.6)

These approximations are good only near the origin. Note that when \( q \) is zero, equation (2.4) becomes the \( p \)-th order Taylor series expansion as follows:

\[
R_{p0}(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots + \frac{z^p}{p!}
\]

(2.7)

The matrix exponential can be expanded in the same way by replacing \( z \) with matrix \( A \). A Taylor series approach to matrix exponential approximation is generally slow and inaccurate. The Padé approximation to the matrix exponential can be computed by simply replacing the \( z \) in equation (2.4); for example, when \( p = q = 2 \), equation (2.4) is written as:

\[
R_{p=2,q=2}(A) = D_{p=2,q=2}(A)^{-1} N_{p=2,q=2}(A),
\]

(2.8)

where

\[
D_{p=2,q=2}(A) = I - \frac{1}{2} A + \frac{1}{12} A^2
\]

(2.9)

and

\[
N_{p=2,q=2}(A) = I + \frac{1}{2} A + \frac{1}{12} A^2
\]

(2.10)

Padé approximation is only accurate near the origin so that the computing procedure should be altered as \( e^A = (e^{A/m})^m \), where \( m \) is a power of 2 to achieve efficiency. It is \( (e^{A/m}) \) that is the first computed. Error can be minimized by choosing equal
p and q values (Golub and Van Loan, [6]).

(IV) Cauchy integral form of matrix functions [11]

Let \( A \in \mathbb{C}^{n \times n} \) be square matrix with eigenvalues \( \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \) then, the matrix function \( f(A) \) defined by:

\[
f(A) = \frac{1}{2\pi i} \oint_{\Gamma} f(z) (zI - A)^{-1} dz
\]

(2.11)

where \( \Gamma \) consists of a finite number of simple closed curves \( \Gamma_k \) with interiors \( \Omega_k \) such that:

1. \( f(z) \) is analytic on \( \Gamma_k \) and on \( \Omega_k \).
2. Each \( \lambda_i \) is contained in some \( \Omega_k \).

(V) M. Dehghan and M. Hajarian, definitions for matrix functions [2]

(a) Let \( A \) be an \((n+1)\) by \((n+1)\) real matrix with distinct real eigenvalues, \( \sigma(A) = \{\lambda_0, \lambda_1, \ldots, \lambda_n\} \) where \( \lambda_0 < \lambda_1 < \cdots < \lambda_n \) and \( f: \mathbb{C} \rightarrow \mathbb{C} \) be defined on the spectrum of \( A(\sigma(A)) \). Now M. Dehghan and M. Hajarian defined \( f(A) \) as follows:

\[
f(A) = \sum_{i=0}^{n} K[\lambda_0, \lambda_1, \ldots, \lambda_i] \prod_{j=0}^{i-1} (A - \lambda_j I),
\]

(2.12)

in which

\[
\begin{align*}
K[\lambda_0] &= f(\lambda_0), \\
K[\lambda_0, \lambda_1] &= \frac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}, \\
K[\lambda_i, \lambda_{i+1}, \ldots, \lambda_{i+k}] &= \frac{f[k](\lambda)}{k!} \\
& \quad \text{if } \lambda_i = \lambda_{i+k} \quad (2.15) \\
& \quad \text{otherwise}
\end{align*}
\]

Note that: \( K[\lambda_0, \lambda_1] \) are Newton’s divided differences, \( f(\lambda_i) I = f(\lambda_i) I \) for \( i = 0, 1, 2, \ldots, n \).

(b) Let \( A \) be an \((n+1)\) by \((n+1)\) real matrix where its eigenvalues are not necessarily distinct, \( \sigma(A) = \{\lambda_0, \lambda_1, \ldots, \lambda_n\} \) where \( \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_n \), and \( f: \mathbb{C} \rightarrow \mathbb{C} \) be defined on the spectrum of \( A(\sigma(A)) \) and \( f(z) \) be a scalar analytic defined function at \( z = \lambda_i \) for \( i = 0, 1, 2, \ldots, n \). Now they defined matrix function \( f(A) \) as follows:

\[
f(A) = \sum_{i=0}^{n} K[\lambda_0, \lambda_1, \ldots, \lambda_i] \prod_{j=0}^{i-1} (A - \lambda_j I),
\]

(2.14)

in which

\[
\begin{align*}
K[\lambda_0, \lambda_1] &= \frac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}, \\
K[\lambda_i, \lambda_{i+1}, \ldots, \lambda_{i+k}] &= \frac{f[k](\lambda)}{k!} \\
& \quad \text{if } \lambda_i = \lambda_{i+k} \quad (2.15) \\
& \quad \text{otherwise}
\end{align*}
\]

Note that: if all eigenvalues of a square matrix \( A \in \mathbb{C}^{n+1 \times n+1} \) are equal to \( \lambda \) then, the matrix function takes the form:

\[
f(A) = f(\lambda) I + f(\lambda) (A - \lambda I)^2 + \frac{f(\lambda)}{2!} (A - \lambda I)^2 + \cdots + \frac{f^{(n)}(\lambda)}{n!} (A - \lambda I)^n.
\]

(2.16)

(VI) M. Dehghan and M. Hajarian, definition for computing matrix functions [3]

Let \( A \) be an \((n+1)\) by \((n+1)\) real matrix with distinct real eigenvalues \( \sigma(A) = \{\lambda_0, \lambda_1, \ldots, \lambda_n\} \) where \( \lambda_0 < \lambda_1 < \cdots < \lambda_n \). Assume that a scalar function \( f \) is defined in a certain domain of the real plane containing the spectrum of \( A(\sigma(A)) \). Now, they defined a matrix function \( f(A) \) by the following form:

\[
f(A) = \alpha G(A) + \beta H(A) + \sum_{i=0}^{n-2} \eta_i A^i,
\]

(2.17)

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where \( \{\alpha, \beta, \eta_0, \eta_1, \ldots, \eta_{n-2}\} \) are obtained from the following conditions:

\[
\begin{align*}
f(\lambda_k) &= f(\lambda_k)I, \quad G(\lambda_k) = G(\lambda_k)I, \quad H(\lambda_k) = H(\lambda_k)I, \quad k = 0, 1, \ldots, n. \quad (2.18)
\end{align*}
\]

The functions \( G \) and \( H \) are given scalar functions defined on \( \sigma(A) \) and the matrix functions \( G(A) \) and \( H(A) \) are computed by the Sylvester’s definition on \( \sigma(A) \) (for more details see [2]).

**Theorem 2.1** [2]: Suppose that \( A \in \mathbb{C}^{n\times n+1} \), \( G(z) = \cos(vz) \), \( (G(A) = \cos(vA)) \), \( H(z) = \sin(vz) \), \( (H(A) = \sin(vA)) \), \( \lambda_0 < \lambda_1 < \cdots < \lambda_n \) and \( 0 < v(\lambda_n - \lambda_0) < \pi \) then, definition VI is well defined.

**Theorem 2.2** [2]: Let \( G(z) = z^{n-1} \ (G(A) = A^{n-1}) \) and \( H(z) = z^n \ (H(A) = A^n) \), then, the definition VI is well defined.

**Theorem 2.3** [7]: If the function \( f(\lambda) \) can be expanded in a power series in the circle \(| \lambda - \lambda_0 | < r \),

\[
f(\lambda) = \sum_{p=0}^{\infty} \alpha_p(\lambda - \lambda_0)^p,
\]

then this expansion remains valid when the scalar argument \( \lambda \) is replaced by a matrix \( A \) whose characteristic values lie within the circle of convergence.

In this theorem we may allow a characteristic value \( \lambda_k \) of \( A \) to fall on the circumference of the circle of convergence; but we must then postulate in addition that the series (2.19), differentiated \((m_k - 1)\) times term by term, should converge at the point \( \lambda = \lambda_k \). It is well known that this already implies the convergence of the \( j \) times differentiated series (2.19) at the point \( \lambda_k \) to \( f^{(j)}(\lambda_k) \) for \( j = 0, 1, \ldots, m_k - 1 \).

The theorem just stated leads, for example, to the following expansions:

\[
\begin{align*}
e^A &= \sum_{p=0}^{\infty} \frac{A^p}{p!}, \quad \cos A = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p)!} A^{2p}, \quad \sin A = \sum_{p=0}^{\infty} \frac{(-1)^p}{(2p+1)!} A^{2p+1},
\end{align*}
\]

\[
\begin{align*}
cosh A &= \sum_{p=0}^{\infty} \frac{A^{2p}}{(2p)!}, \quad \sinh A = \sum_{p=0}^{\infty} \frac{A^{2p+1}}{(2p+1)!},
\end{align*}
\]

\[
\begin{align*}(I - A)^{-1} &= \sum_{p=0}^{\infty} A^p, \quad (|\lambda_k| < 1 \ ; \ k = 1, 2, \ldots, s),
\end{align*}
\]

\[
\begin{align*}\ln A &= \sum_{p=0}^{\infty} \frac{(-1)^{p-1}}{p} (A - I)^p, \quad (|\lambda_k - 1| < 1 \ ; \ k = 1, 2, \ldots, s).
\end{align*}
\]

(By \( \ln \lambda \), we mean here the so-called principal value of the many-valued function \( \ln \lambda \) that is the branch for which \( \ln 1 = 0 \).

### 3 Main results

In this section we introduce the main results of our definition and theorems. The definition VI and Theorems 2.1, 2.2 are used to help us to state our definition and prove our theorems.

**Definition 3.1** (Matrix functions using numerical hybrid method) Let \( A \in \mathbb{C}^{n\times n} \) be a square matrix with mixed eigenvalues (distinct real and complex). That is its spectrum has the form:

\( \sigma(A) = \{\lambda_0, \lambda_1, \ldots, \lambda_k, \lambda_{k+1}, \ldots, \lambda_{k+n-1}, \lambda_{k+n-1}\} \) where \( n \geq 3 \), \( n \) odd positive integer number, \( 0 \leq k \leq n - 3 \) and \( \frac{k+n-1}{2} \) is positive integer number). Suppose that \( f \) is a scalar function defined on a certain domain of complex plane containing the spectrum of \( A (\sigma(A)) \). Now, we define the matrix function \( f(A) \) by the form:

\[
f(A) = \alpha G(A) + \beta H(A) + \sum_{i=0}^{n-3} \eta_i A^i,
\]

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where \( \{ \alpha, \beta, \eta_0, \eta_1, \ldots, \eta_{n-3} \} \) are obtained by the following conditions:

\[
\begin{align*}
f(\lambda_k I) &= f(\lambda_k I), \quad G(\lambda_k I) = G(\lambda_k I), \quad H(\lambda_k I) = H(\lambda_k I), \\
f(\lambda_m I) &= f(\lambda_m I), \quad G(\lambda_m I) = G(\lambda_m I), \quad H(\lambda_m I) = H(\lambda_m I), \\
f(\lambda_{m+1} I) &= f(\lambda_{m+1} I), \quad G(\lambda_{m+1} I) = G(\lambda_{m+1} I), \quad H(\lambda_{m+1} I) = H(\lambda_{m+1} I), \\
\text{for } k &= 0, 1, \ldots, n-3 \text{ and } m = k + 1, \ldots, \frac{k+n-1}{2},
\end{align*}
\]

(3.2)

G and H are given scalar functions defined on \( \sigma(A) \) and the matrix functions \( G(A) \) and \( H(A) \) are computed using extension of Sylvester definition for computing matrix functions.

**Theorem 3.1** Suppose that \( G(z) = \cos(vz) \), \( (G(A) = \cos(vA)) \), \( H(z) = \sin(vz) \), \( (H(A) = \sin(vA)) \) and \( \sigma(A) = \{ \lambda_0, \lambda_1, \ldots, \lambda_k, \lambda_{k+1}, \ldots, \lambda_{k+n-1}, \lambda_{k+n-1} \} \) is ordered as:

1. The real eigenvalues should satisfy \( 0 < \lambda_0 < \lambda_1 < \cdots < \lambda_k \text{ and } 0 < v(\lambda_k - \lambda_0) < \pi, \) where \( v \) is a positive real parameter.

2. The complex eigenvalues should also satisfy:

\[
Re \lambda_{k+1} \leq Re \lambda_{k+2} \leq \cdots \leq Re \lambda_{k+n-1} \leq Re \lambda_{k+n-1}, 0 < v \left( Re \lambda_{k+n-1} - Re \lambda_{k+1} \right) < \pi, \text{ where } v \text{ is a positive real parameter. Then, definition 3.1 is well defined.}
\]

Remarks:

1. If the square matrix \( A \) having only one real eigenvalue (\( k = 0 \)) in this case it should satisfy \( 0 < v\lambda_0 < \pi. \)

2. If the square matrix \( A \) having only one complex eigenvalue in this case it should satisfy \( 0 < vRe \lambda_{k+1} < \pi \)

**Proof.** We first, from the definition 3.1, the matrix functions \( G(A) \) and \( H(A) \) are computed by a definition which satisfy the conditions in (3.2). Now, we show that the unique coefficients \( \{ \alpha, \beta, \eta_0, \eta_1, \ldots, \eta_{n-3} \} \) are existed for \( G(z) = \cos(vz) \), \( (G(A) = \cos(vA)) \), \( H(z) = \sin(vz) \), \( (H(A) = \sin(vA)) \). Using these coefficients then, the matrix function \( f(A) \) can be computed. Now, by considering the conditions (3.2), then substitute in (3.1), we have:

\[
f(\lambda_k I) = f(\lambda_k I) = \alpha G(\lambda_k I) + \beta H(\lambda_k I) + \sum_{i=0}^{n-3} \eta_i (\lambda_k I)^i = \alpha G(\lambda_k I) + \beta H(\lambda_k I) + \sum_{i=0}^{n-3} \eta_i (\lambda_k)^i I
\]

\[
= \left[ \alpha G(\lambda_k) + \beta H(\lambda_k) + \sum_{i=0}^{n-3} \eta_i (\lambda_k)^i \right] I,
\]

(3.1)

\[
f(\lambda_m I) = f(\lambda_m I) = \alpha G(\lambda_m I) + \beta H(\lambda_m I) + \sum_{i=0}^{n-3} \eta_i (\lambda_m I)^i = \alpha G(\lambda_m I) + \beta H(\lambda_m I) + \sum_{i=0}^{n-3} \eta_i (\lambda_m)^i I
\]

\[
= \left[ \alpha G(\lambda_m) + \beta H(\lambda_m) + \sum_{i=0}^{n-3} \eta_i (\lambda_m)^i \right] I,
\]

(3.2)

\[
f(\lambda_{m+1} I) = f(\lambda_{m+1} I) = \alpha G(\lambda_{m+1} I) + \beta H(\lambda_{m+1} I) + \sum_{i=0}^{n-3} \eta_i (\lambda_{m+1} I)^i = \alpha G(\lambda_{m+1} I) + \beta H(\lambda_{m+1} I) + \sum_{i=0}^{n-3} \eta_i (\lambda_{m+1})^i I
\]

\[
= \left[ \alpha G(\lambda_{m+1}) + \beta H(\lambda_{m+1}) + \sum_{i=0}^{n-3} \eta_i (\lambda_{m+1})^i \right] I,
\]

(3.3)
fork = 0, 1, ⋯, n - 3 and m = k + 1, ⋯, \frac{k+n-1}{2}. This implies that:

\[
\begin{align*}
\alpha G(\lambda_0) + \beta H(\lambda_0) + \sum_{i=0}^{n-3} \eta_i(\lambda_0)^i &= f(\lambda_0); \\
\alpha G(\lambda_1) + \beta H(\lambda_1) + \sum_{i=0}^{n-3} \eta_i(\lambda_1)^i &= f(\lambda_1); \\
&\cdots \\
\alpha G(\lambda_{k+1}) + \beta H(\lambda_{k+1}) + \sum_{i=0}^{n-3} \eta_i(\lambda_{k+1})^i &= f(\lambda_{k+1}); \\
\alpha G(\lambda_{k+n-1}) + \beta H(\lambda_{k+n-1}) + \sum_{i=0}^{n-3} \eta_i(\lambda_{k+n-1})^i &= f(\lambda_{k+n-1}); \\
\end{align*}
\]  

(3.4)

The above linear system can be written as in the following form:

\[
BX = C
\]

(3.5)

where

\[
B = \begin{pmatrix}
G(\lambda_0) & H(\lambda_0) & 1 & \lambda_0 & \lambda_0^2 & \cdots & \lambda_0^{n-3} \\
G(\lambda_1) & H(\lambda_1) & 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{n-3} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
G(\lambda_k) & H(\lambda_k) & 1 & \lambda_k & \lambda_k^2 & \cdots & \lambda_k^{n-3} \\
G(\lambda_{k+1}) & H(\lambda_{k+1}) & 1 & \lambda_{k+1} & \lambda_{k+1}^2 & \cdots & \lambda_{k+1}^{n-3} \\
G(\lambda_{k+n-1}) & H(\lambda_{k+n-1}) & 1 & \lambda_{k+n-1} & \lambda_{k+n-1}^2 & \cdots & \lambda_{k+n-1}^{n-3} \\
\end{pmatrix}
\]

\[
X = (\alpha, \beta, \eta_0, \eta_1, \cdots, \eta_{n-3})^T
\]

and

\[
C = \left( f(\lambda_0), f(\lambda_1), \ldots, f(\lambda_{k+1}), f(\lambda_{k+n-1}), \ldots, f(\lambda_{k+n-1}), f(\lambda_{k+n-1}) \right)^T
\]

(3.6)

Now, we compute determinant of B and prove it is not equal to zero, as follows: Since,

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where \((n \geq 3, n\) odd number, \(0 \leq k \leq n - 3\) and \(\frac{k + n - 1}{2}\) is a positive integer number). Also note that \(n\) is the number of all eigenvalues of matrix \(A\) and \(k\) refers to the index of real eigenvalues (number of real eigenvalues equal to \((k + 1)\). The process of computing \(\det (B)\) can be discussed through the following:

**Step 1:** Let \(A \in \mathbb{C}^{3 \times 3}\) be a square matrix of three eigenvalues where one of them is real while the other is complex eigenvalue with its complex conjugate. Let \(\lambda_0\) be real and \(\lambda_1\) be complex eigenvalue (with its complex conjugate \(\bar{\lambda}_1\)) then,

\[
\det (B) = \begin{bmatrix}
G(\lambda_0) & H(\lambda_0) & 1 & \lambda_0 & \lambda_0^2 & \cdots & \lambda_0^{n-3} \\
G(\lambda_1) & H(\lambda_1) & 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^{n-3} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
G(\lambda_k) & H(\lambda_k) & 1 & \lambda_k & \lambda_k^2 & \cdots & \lambda_k^{n-3} \\
G(\lambda_{k+1}) & H(\lambda_{k+1}) & 1 & \lambda_{k+1} & \lambda_{k+1}^2 & \cdots & \lambda_{k+1}^{n-3} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
G(\lambda_{\frac{k+n-1}{2}}) & H(\lambda_{\frac{k+n-1}{2}}) & 1 & \lambda_{\frac{k+n-1}{2}} & \lambda_{\frac{k+n-1}{2}}^2 & \cdots & \lambda_{\frac{k+n-1}{2}}^{n-3} \\
\end{bmatrix} (3.7)
\]

**Step 2:** Let \(A \in \mathbb{C}^{5 \times 5}\) be a square matrix having five eigenvalues. Then, there are two possible cases to be discussed as follows:

Case a: There are three real eigenvalues and one complex eigenvalue with its complex conjugate.

Case b: There is only one real eigenvalue and two complex eigenvalues with their complex conjugates)

For case a: Suppose eigenvalues of \(A\) having the form:

\(\lambda_0, \lambda_1 \) and \(\lambda_2\) (are positive real numbers), \(\lambda_3\) and \(\bar{\lambda}_3\) (are complex) now, using conditions in Eq. \((3.2)\) then, we have:

\[
\det (B) = (\lambda_1 - \lambda_0) (\lambda_2 - \lambda_0) (\lambda_3 - \lambda_0) (\bar{\lambda}_3 - \lambda_0) \begin{bmatrix}
G(\lambda_0) & H(\lambda_0) & 1 & \lambda_0 & \lambda_0^2 \\
G(\lambda_1) & H(\lambda_1) & 1 & \lambda_1 & \lambda_1^2 \\
G(\lambda_2) & H(\lambda_2) & 1 & \lambda_2 & \lambda_2^2 \\
G(\lambda_3) & H(\lambda_3) & 1 & \lambda_3 & \lambda_3^2 \\
G(\bar{\lambda}_3) & H(\bar{\lambda}_3) & 1 & \bar{\lambda}_3 & \bar{\lambda}_3^2 \\
\end{bmatrix} (3.11)
\]

Using remarks in our theorem and Eq. \((3.10)\) then, we have \(\det (B)\) does not vanish.

**Case a:** There are three real eigenvalues and one complex eigenvalue with its complex conjugate.

**Case b:** There is only one real eigenvalue and two complex eigenvalues with their complex conjugates.

Set: \( D = (\lambda_1 - \lambda_0)(\lambda_2 - \lambda_0)(\lambda_3 - \lambda_0)(\bar{\lambda}_3 - \lambda_0) \) then, we have:

\[
\det(B) = D \begin{vmatrix}
G(\lambda_0) & H(\lambda_0) & 1 & \lambda_0 & 0 \\
G[\lambda_1, \lambda_0] & H[\lambda_1, \lambda_0] & 0 & 1 & \lambda_1 \\
G[\lambda_2, \lambda_0] & H[\lambda_2, \lambda_0] & 0 & 1 & \lambda_2 \\
G[\lambda_3, \lambda_0] & H[\lambda_3, \lambda_0] & 0 & 1 & \lambda_3 \\
G[\bar{\lambda}_3, \lambda_0] & H[\bar{\lambda}_3, \lambda_0] & 0 & 1 & \bar{\lambda}_3 \\
\end{vmatrix} + D \begin{vmatrix}
G(\lambda_0) & H(\lambda_0) & 1 & \lambda_0 & 0 \\
G[\lambda_1, \lambda_0] & H[\lambda_1, \lambda_0] & 0 & 1 & \lambda_0 \\
G[\lambda_2, \lambda_0] & H[\lambda_2, \lambda_0] & 0 & 1 & \lambda_0 \\
G[\lambda_3, \lambda_0] & H[\lambda_3, \lambda_0] & 0 & 1 & \lambda_0 \\
G[\bar{\lambda}_3, \lambda_0] & H[\bar{\lambda}_3, \lambda_0] & 0 & 1 & \bar{\lambda}_3 \\
\end{vmatrix} = D \begin{vmatrix}
G[\lambda_1, \lambda_0] & H[\lambda_1, \lambda_0] & 1 & \lambda_1 \\
G[\lambda_2, \lambda_0] - G[\lambda_1, \lambda_0] & H[\lambda_2, \lambda_0] - H[\lambda_1, \lambda_0] & 0 & \lambda_2 - \lambda_1 \\
G[\lambda_3, \lambda_0] - G[\lambda_1, \lambda_0] & H[\lambda_3, \lambda_0] - H[\lambda_1, \lambda_0] & 0 & \lambda_3 - \lambda_1 \\
G[\bar{\lambda}_3, \lambda_0] - G[\lambda_1, \lambda_0] & H[\bar{\lambda}_3, \lambda_0] - H[\lambda_1, \lambda_0] & 0 & \bar{\lambda}_3 - \lambda_1 \\
\end{vmatrix}
\]

(3.12)

Also, set \( W = (\lambda_2 - \lambda_1)(\lambda_3 - \lambda_1)(\bar{\lambda}_3 - \lambda_1) \) then, we have:

\[
\det(B) = DW \begin{vmatrix}
G[\lambda_1, \lambda_0, \lambda_2] & H[\lambda_1, \lambda_0, \lambda_2] & 1 \\
G[\lambda_1, \lambda_0, \lambda_3] & H[\lambda_1, \lambda_0, \lambda_3] & 1 \\
G[\lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_1, \lambda_0, \bar{\lambda}_3] & 1 \\
\end{vmatrix}
\]

(3.13)

Finally,

\[
\det(B) = DW \begin{vmatrix}
G[\lambda_1, \lambda_0, \lambda_2] & H[\lambda_1, \lambda_0, \lambda_2] & 1 \\
G[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & H[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & 1 \\
G[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & 1 \\
\end{vmatrix}
\]

(3.14)

Since, \( D = (\lambda_1 - \lambda_0)(\lambda_2 - \lambda_0)(\lambda_3 - \lambda_0)(\bar{\lambda}_3 - \lambda_0) \) and \( W = (\lambda_2 - \lambda_1)(\lambda_3 - \lambda_1)(\bar{\lambda}_3 - \lambda_1) \) then, we have:

\[
\det(B) = (\lambda_1 - \lambda_0)(\lambda_2 - \lambda_0)(\lambda_3 - \lambda_0)(\bar{\lambda}_3 - \lambda_0)(\lambda_2 - \lambda_1)(\lambda_3 - \lambda_1)(\bar{\lambda}_3 - \lambda_1)(\lambda_3 - \lambda_2)(\bar{\lambda}_3 - \lambda_2) \times \begin{vmatrix}
G[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & H[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & 0 \\
G[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & 0 \\
G[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & 0 \\
\end{vmatrix}
\]

(3.15)

Hence,

\[
\det(B) = D \prod_{i=1, j<i}^{3} (\lambda_i - \lambda_j) \prod_{s=0}^{2} (\bar{\lambda}_3 - \lambda_s) \begin{vmatrix}
G[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & H[\lambda_2, \lambda_1, \lambda_0, \lambda_3] & 0 \\
G[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & 0 \\
G[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & H[\lambda_2, \lambda_1, \lambda_0, \bar{\lambda}_3] & 0 \\
\end{vmatrix}
\]

(3.16)

where \( j = 0, 1, \ldots, i - 1 \) and \( s = 0, 1, 2 \).

For case b: Suppose eigenvalues of \( A \) having the form: \( \lambda_0 \) (is a positive real eigenvalue), \( \lambda_1, \lambda_2 \) and \( \bar{\lambda}_1, \bar{\lambda}_2 \) (are complex eigenvalues with their complex conjugates) respectively now, using conditions in Eq. (3.2) then, we have:

\[
\det(B) = \prod_{i=1, j<i}^{2} (\lambda_i - \lambda_j)(\bar{\lambda}_i - \lambda_j) \prod_{r=1}^{2} (\lambda_r - \lambda_j) \prod_{s=2, 0 < t < s} (\bar{\lambda}_s - \bar{\lambda}_t)(\bar{\lambda}_s - \lambda_t) \begin{vmatrix}
G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] & G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] & \cdots & G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] \\
G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] & G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] & \cdots & G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] \\
\end{vmatrix}
\]

(3.17)

Hence, from steps 1 and 2 we deduce that the value of \( \det(B) \) can be given in the following three different forms depending on the types of the set of eigenvalues of a square matrix \( A \).

\[
H[\lambda_0, \lambda_1, \bar{\lambda}_1, \cdots, \bar{\lambda}_2, \bar{\lambda}_2] = \begin{vmatrix}
G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] & G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] & \cdots & G[\lambda_0, \lambda_1, \lambda_2, \bar{\lambda}_1, \bar{\lambda}_2] \\
G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] & G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] & \cdots & G[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \bar{\lambda}_1, \bar{\lambda}_2] \\
\end{vmatrix}
\]

(3.18)

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Form 1: If the square matrix $A$ having only one complex eigenvalue with its complex conjugate and the remainder eigenvalues are real then, we have:

$$
\det (B) = \prod_{i=1,j<i}^{n-2} (\lambda_i - \lambda_j) \prod_{s=0}^{n-3} (\bar{\lambda}_{n-2} - \lambda_s) \{G[\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{k-1}]H[\lambda_0, \lambda_1, \ldots, \lambda_k, \bar{\lambda}_{n-2}] - H[\lambda_0, \lambda_1, \ldots, \lambda_k, \bar{\lambda}_{n-2}]G[\lambda_0, \lambda_1, \ldots, \lambda_k, \bar{\lambda}_{n-2}]\}
$$

(3.19)

where in this case $n \geq 3$, $j = 0, 1, 2, \ldots, i - 1$ and $s, k = 0, 1, \ldots, n - 3$.

Form 2: If the square matrix $A$ having only three real eigenvalues $\lambda_0$, $\lambda_1$, $\lambda_2$ and the remainder eigenvalues are complex then, we have:

$$
\det (B) = \prod_{i=1,j<i}^{n-4} (\lambda_i - \lambda_j) \prod_{r=1}^{n-4} (\bar{\lambda}_{n-4} - \lambda_r) \prod_{m=0}^{n-3} (\bar{\lambda}_{n-2} - \lambda_m) \times \\
\prod_{s=4}^{n-3} (\lambda_s - \bar{\lambda}_t) (\bar{\lambda}_s - \bar{\lambda}_t)\{G[\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{m-1}, \lambda_{m+1}] - H[\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{m-1}, \lambda_{m+1}]G[\lambda_0, \lambda_1, \ldots, \lambda_{m-1}, \lambda_{m+1}]\}
$$

(3.20)

where in this case $n \geq 7$, $j = 0, 1, \ldots, i - 1$, $r = 1, 3, \ldots, n - 4$ and $m = 0, 1, \ldots, n - 4$.

Remark: For $n = 5$ we have form 1.

Form 3: If the square matrix $A$ having only one real eigenvalue and the remainder eigenvalues are complex with their complex conjugates then, we have:

$$
\det (B) = \prod_{i=1,j<i}^{n-1} (\lambda_i - \lambda_j) (\bar{\lambda}_i - \lambda_j) \prod_{r=1}^{n-1} (\bar{\lambda}_r - \lambda_r) \prod_{s=2}^{n-3} (\lambda_s - \bar{\lambda}_t) (\bar{\lambda}_s - \bar{\lambda}_t) \{G[\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{m-1}, \lambda_{m+1}] - H[\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_{m-1}, \lambda_{m+1}]G[\lambda_0, \lambda_1, \ldots, \lambda_{m-1}, \lambda_{m+1}]\}
$$

(3.21)

where $n \geq 5$, $j = 0, 1, \ldots, i - 1$. Now, the previous forms 1, 2 and 3 can be rewritten in the following short forms:

For Form 1:

$$
\det (B) = \prod_{i=1,j<i}^{n-2} (\lambda_i - \lambda_j) \prod_{s=0}^{n-3} (\bar{\lambda}_{n-2} - \lambda_s) \{G[\sigma_n]H(\sigma_{n-1}) - H(\sigma_n)G(\sigma_{n-1})\}
$$

(3.22)

For Form 2:

$$
\det (B) = \prod_{i=1,j<i}^{n+1} (\lambda_i - \lambda_j) \prod_{r=1}^{n-4} (\bar{\lambda}_{n-4} - \lambda_r) \prod_{m=0}^{n-3} (\bar{\lambda}_{n-2} - \lambda_m) \times \\
\prod_{s=4}^{n-3} (\lambda_s - \bar{\lambda}_t) (\bar{\lambda}_s - \bar{\lambda}_t) \{G[\sigma_n]H(\sigma_{n-1}) - H(\sigma_n)G(\sigma_{n-1})\}
$$

(3.23)
For Form 3:

\[
\det(B) = \prod_{i=1}^{n-1} (\lambda_i - \lambda_j) \prod_{r=1}^{n-3} (\bar{\lambda}_r - \lambda_r) \times \\
\prod_{s=2}^{n-1} (\lambda_s - \bar{\lambda}_s) (\bar{\lambda}_s - \bar{\lambda}_r) \{G(\sigma_n) H(\sigma_n) - H(\sigma_n) G(\sigma_n)\} \\
\begin{cases}
\text{for } 0 < t < s \\
\text{0 otherwise}
\end{cases}
\]

(3.24)

where \( \sigma_n \equiv \sigma_n(A) \), \( \sigma_n-1 \equiv \sigma_n-1(A) \). In general, we denote \( \sigma_n \) to be the set of interpolation nodes which does not contain the last eigenvalue and \( \sigma_n-1 \) be the set of interpolation nodes obtained by removing the node before last eigenvalue and contains last eigenvalue. Also \( n \geq 3, n \) odd positive integer number which refer to the number of all eigenvalues of a square matrix \( A \), \( 0 \leq k \leq n-3 \) which refers to the index of the real eigenvalues where number of real eigenvalues equal to \( (k+1) \), \( \bar{\lambda}_{k+1} \) refers to the eigenvalue number \( n \) (last eigenvalue) and \( -\frac{k+n-1}{2} \) positive integer number. Now, we need to prove that \( \det(B) \neq 0 \). Since, from Form 3, we have:

\[
\det(B) = \prod_{i=1}^{n-1} (\lambda_i - \lambda_j) \prod_{r=1}^{n-3} (\bar{\lambda}_r - \lambda_r) \times \\
\prod_{s=2}^{n-1} (\lambda_s - \bar{\lambda}_s) (\bar{\lambda}_s - \bar{\lambda}_r) \{G(\sigma_n) H(\sigma_n) - H(\sigma_n) G(\sigma_n)\} \\
\begin{cases}
\text{for } 0 < t < s \\
\text{0 otherwise}
\end{cases}
\]

(3.25)

and using results in [1, 3], extension of Sylvester definition for computing the terms of \( \{G(\sigma_n) H(\sigma_n) - H(\sigma_n) G(\sigma_n)\} \) and the assumptions \( 0 < \lambda_0 \nu < \pi \) and \( 0 < \nu \left( \text{Re}\sum_{i=1}^{n-1} \lambda_i - \text{Re}\lambda_1 \right) < \pi \) as in our Theorem 3.1 then, we can show that \( \det(B) \neq 0 \) where we use the known value of the Vandermonde determinant with \( G(\nu) = \cos(\nu \lambda) \) and \( H(\lambda) = \sin(\nu \lambda) \). Therefore, there exist unique coefficients \( \{\alpha, \beta, \eta_0, \eta_1, \ldots, \eta_{n-3}\} \). This implies that definition 3.1 is well defined for \( (G(A) = \cos(\nu A) \) and \( H(A) = \sin(\nu A) \). Now the proof of our theorem is complete.\]  

Note: if we use form 1 or form 2 for the determinant of \( B \) where \( \det(B) \) as in Eq. (3.22) or as in Eq. (3.23) we get the same result that is \( \det(B) \neq 0 \).

**In particular case let \( n=3 \):** Let \( A \in \mathbb{C}^{3 \times 3} \) be a square matrix of three eigenvalues where one of them is real while the other is complex eigenvalue with its complex conjugate. Let these eigenvalues have the following form:

\( \lambda_0 = \alpha_0, \lambda_1 = \alpha_1 + i\beta_1 \) and \( \bar{\lambda}_1 = \alpha_1 - i\beta_1, \alpha_0, \alpha_1 \) and \( \beta_1 \) are positive real numbers and \( \alpha_0 \neq \alpha_1 \). Now, using [1] and our technique we have:

\[
\det(B) = \sin(v(\bar{\lambda}_1 - \lambda_1)) + \sin(v(\lambda_1 - \lambda_0)) + \sin(v(\lambda_0 - \bar{\lambda}_1)) \\
= 4\sin\left(\frac{v(\bar{\lambda}_1 - \lambda_1)}{2}\right) \sin\left(\frac{v(\lambda_1 - \lambda_0)}{2}\right) \sin\left(\frac{v(\lambda_0 - \bar{\lambda}_1)}{2}\right)
\]

(3.26)

In this case we prove \( \det(B) \neq 0 \) as follows:

\[
\det(B) = 4\sin(v(-i\beta_1))\sin\left(\frac{v((\alpha_1 - \alpha_0) + i\beta_1)}{2}\right) \sin\left(\frac{v((\alpha_1 - \alpha_0) - i\beta_1)}{2}\right) \\
= -4\sinh(v\beta_1) \left\{ \sin\left(\frac{v(\alpha_1 - \alpha_0)}{2}\right) \cos\left(\frac{iv\beta_1}{2}\right) + \cos\left(\frac{v(\alpha_1 - \alpha_0)}{2}\right) \sin\left(\frac{iv\beta_1}{2}\right) \right\} \\
\times \left\{ \sin\left(\frac{v(\alpha_1 - \alpha_0)}{2}\right) \cos\left(\frac{iv\beta_1}{2}\right) - \cos\left(\frac{v(\alpha_1 - \alpha_0)}{2}\right) \sin\left(\frac{iv\beta_1}{2}\right) \right\}
\]

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Since
Assume that:

\[ 0 \leq \partial_0 \leq 1, \quad \Re \lambda_0 = 0, \quad \Re \lambda_1 = \Re \lambda_1 = \frac{1}{2} \]

Now Eq. (3.22) yield

\[ \det(B) = \prod_{i=1, j<i}^{n-2} (\lambda_i - \lambda_j) \prod_{s=0}^{n-3} (\lambda_{n-2} - \lambda_s) (\lambda_1 + \lambda_1) \neq 0. \]

The proof is completed. \( \blacksquare \)

Note: This theorem is the same as Theorem 2.1 in [3] so that the proof of it is as the same as in [2] with small different calculation in our theorem so, we follow the same technique of the proof of Theorem 3.1. This theorem is used in our examples to compute matrix functions \( f(A) \). Polar coordinates should used to find the functions of complex eigenvalues.

### 4 Numerical examples

In this section, we give several different examples to validate our theoretical results and to illustrate the applicability of the presented technique and to show that this technique gives high accuracy for computing matrix functions \( f(A) \). Polar coordinates is used for computation of the functions of the complex eigenvalues.

**Example 4.1** Let \( A = \begin{pmatrix} 1 & -2 & 0 \\ 4 & 1 & 2 \\ 2 & 3 & 2 \end{pmatrix} \in \mathbb{C}^{3 \times 3} \) and \( f(z) = \sqrt{z} \) then compute \( f(A) \).

First: it is easy to note that: \( \sigma(A) = \left\{ 1_2 + \frac{\sqrt{2}}{2}, \frac{3}{2}, 2 \right\} \)

Assume that:\n\( \lambda_0 = 1, \quad \lambda_1 = \frac{1}{2} + \frac{\sqrt{2}}{2} i, \quad \lambda_1 = \frac{1}{2} - \frac{\sqrt{2}}{2} i \)

Since \( 0 < \lambda_0, \quad \Re \lambda_1 \leq \Re \lambda_1 \) then, definition 3.1 can be applied for this example, hence, we have:

\[ f(A) = \alpha G(A) + \beta H(A) + \eta_0 I = \alpha A + \beta A^2 + \eta_0 I \quad (4.1) \]

where, we suppose the scalar functions defined on the spectrum of \( A \) by \( G(z) = z \) and \( H(z) = z^2 \). Now, the constants \( \alpha, \beta \) and \( \eta_0 \) can be found by using the conditions (3.5) which are equivalent to

\[ \begin{pmatrix} G(\lambda_0) & H(\lambda_0) \\ G(\lambda_1) & H(\lambda_1) \\ G(\lambda_1) & H(\lambda_1) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \eta_0 \end{pmatrix} = \begin{pmatrix} f(\lambda_0) \\ f(\lambda_1) \\ f(\lambda_1) \end{pmatrix} \quad (4.2) \]

\( G(\lambda_i), \quad H(\lambda_i), \quad f(\lambda_i), \quad i = 0, 1 \) and \( G(\lambda_i), \quad H(\lambda_i), \quad f(\lambda_i) \) will be first found then substitute in (4.2) to compute the constants \( \alpha, \beta \) and \( \eta_0 \). Now, (4.2) can be rewritten as:

\[ \begin{pmatrix} 1.5' + 1.322875655322954' + 0.5 i \\ 1.5' - 1.322875655322954' + 0.5' - 3.9686269665968686' i \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \eta_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (4.3) \]

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Solving this linear system of equations (4.3), one can obtain:

\[ \alpha = 0.578805 + 1.11022 \times 10^{-16}i, \quad \beta = -0.0669467 - 2.08167 \times 10^{-17}i \quad \text{and} \quad \eta_0 = 0.488142 - 6.90598 \times 10^{-17}i \]  

(4.4)

Substitute from (4.4) in (4.1), we can obtain:

\[
f(A) = \sqrt{A} = \left\{ \begin{array}{ll}
1.53557 + 1.876 \times 10^{-16}i, & -0.8898 - 1.387 \times 10^{-16}i, 0.26778 + 8.32 \times 10^{-17}i \\
1.5118 + 1.942 \times 10^{-16}i, & 1.13389 + 6.277 \times 10^{-17}i, 0.755929 + 9.714 \times 10^{-17}i \\
-0.0474316 - 1.526 \times 10^{-16}i, & 1.40168 + 2.2898 \times 10^{-17}i, 0.976284 - 5.5182 \times 10^{-17}i \\
\end{array} \right\}
\]

Then,

\[
(f(A))^2 = \left( \sqrt{A} \right)^2 = \sqrt{A} \cdot \sqrt{A}
\]

Since \( f(A) = \sqrt{A} \). Then, \( (f(A))^2 = \left( \sqrt{A} \right)^2 = \sqrt{A} \cdot \sqrt{A} \)

Hence, we can test our result as follows:

\[
(f(A))^2 = \begin{pmatrix} 1 & -2 & 0 \\ 4 & 1 & 2 \\ 2 & 3 & 2 \end{pmatrix} = A
\]

This implies that \( \left( \sqrt{A} \right)^2 = A \). The error approximately 3.88650 \times 10^{-16} therefore, our technique which proposed in definition 3.1 which is proved by our Theorem 3.1 can be used practically and accurately for computing the square root of square matrices having mixed eigenvalues.

Example 4.2 Let \( A = \begin{pmatrix} 1 & -2 & 0 \\ 4 & 1 & 0 \\ 0 & 1 & 4 \end{pmatrix} \in \mathbb{C}^{3 \times 3} \) and \( f(z) = \sqrt{z} \) then compute \( f(A) \).

First: it is easy to note that: \( \sigma(A) = \{ 4, 1 + 2i, 1 - 2i \} \)

Assume that: \( \lambda_0 = 4, \quad \lambda_1 = 1 + 2i, \quad \lambda_1 = 1 - 2i \)

Since \( 0 < v \lambda_0 < \pi, \quad 0 < \text{Re}(v \lambda_1) \leq \pi \) where \( v = \frac{\pi}{\sqrt{2}} \) then, definition 3.1 and Theorem 3.1 can be applied for this example, hence, we have:

\[
f(A) = \alpha G(A) + \beta H(A) + \eta_0 I = \alpha \cos(A) + \beta \sin(A) + \eta_0 I
\]

(4.5)

where, we suppose the scalar functions defined on the spectrum of \( A \) by \( G(z) = \cos(vz) \) and \( H(z) = \sin(vz) \). Now, the constants \( \alpha, \beta \) and \( \eta_0 \) can be found by using the conditions 3.5 which are equivalent to:

\[
\begin{pmatrix}
G(\lambda_0) & H(\lambda_0) & 1 \\
G(\lambda_1) & H(\lambda_1) & 1 \\
G(\lambda_1) & H(\lambda_1) & 1
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta \\
\eta_0
\end{pmatrix}
= 
\begin{pmatrix}
f(\lambda_0) \\
f(\lambda_1) \\
f(\lambda_1)
\end{pmatrix}
\]

(4.6)

Using \( G(\lambda_i), \quad H(\lambda_i), \quad f(\lambda_i), \quad i = 0, 1 \) and \( G(\lambda_1), \quad H(\lambda_1), \quad f(\lambda_1) \) as we supposed then (4.6) rewritten as:

\[
\begin{pmatrix}
\cos(v \lambda_0) & \sin(v \lambda_0) & 1 \\
\cos(v \lambda_1) & \sin(v \lambda_1) & 1 \\
\cos(v \lambda_1) & \sin(v \lambda_1) & 1
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta \\
\eta_0
\end{pmatrix}
= 
\begin{pmatrix}
\sqrt{\lambda_0} \\
\sqrt{\lambda_1} \\
\sqrt{\lambda_1}
\end{pmatrix}
\]

(4.7)

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Find each term in Eq. (4.7) we can obtain the following system:

\[
\begin{pmatrix}
-0.9888308262251285' \\
1.17820312519'i - 4.14188364887'i \\
1.17820312519'i + 4.14188364887'i
\end{pmatrix} =
\begin{pmatrix}
0.14904226617617472' \\
1.59425951780' + 4.15398099493'i \\
1.59425951780' - 4.15398099493'i
\end{pmatrix} \begin{pmatrix}
\alpha \\
\beta \\
\eta_0
\end{pmatrix}
\]

\[
= \begin{pmatrix}
1.272019649514069' + 0.7861513777547233'i \\
1.272019649514069' - 0.7861513777547233'i
\end{pmatrix}
\]

(4.8)

Solving this linear system of equations in (4.8), one can obtain:

\[
\alpha = -0.3604517858518196', \quad \beta = (0.17144472319629234' - 2.77555756156289114' \times 10^{-17} i), \\
\eta_0 = (1.6180216527126996' - 2.7098706138914066' \times 10^{-17} i)
\]

(4.9)

Now, we find the matrix functions \( \cos(A) \) and \( \sin(A) \) using extension of Sylvester definition

\[
\cos (A) = \begin{pmatrix}
1.7182031251913887' \\
-1.441883648876892' \\
-0.8465283936307948'
\end{pmatrix}
\]

(4.10)

and

\[
\sin (A) = \begin{pmatrix}
1.59425951780296966' \\
-1.5539809943636314' \\
-0.99437674231314'
\end{pmatrix}
\]

(4.11)

Now, substitute from Eqs. (4.11), (4.10) and (4.9) in Eq. (4.5), we can obtain the square root of a matrix \( A \) as follows:

\[
f (A) = \sqrt{A}
\]

\[
= \begin{pmatrix}
1.27202 - 7.13483 \times 10^{-17} i & -0.786151 + 4.3131 \times 10^{-17} i & 0 \\
0.7861 - 4.3131 \times 10^{-17} i & 1.27202 - 7.13482 \times 10^{-17} i & 0 \\
0.28894 + 2.6211 \times 10^{-18} i & 1.665 \times 10^{-16} - 4.947 \times 10^{-17} i & 4. - 1.249 \times 10^{-16} i
\end{pmatrix}
\]

Since \( f (A) \) the error is very small and this implies our technique for computing matrix functions of square matrices having mixed eigenvalues using numerical hybrid technique (method in definition 3.1) is applicable and gives high accuracy.

Example 4.3 Consider a square matrix \( A = \begin{pmatrix}
1 & -2 & 0 \\
4 & 1 & 2 \\
2 & 3 & 2
\end{pmatrix} \in \mathbb{C}^{3 \times 3}, f (z) = e^z \) then compute \( f (A) \).

Similarly to Example 4.1, the spectrum of \( A \) can be obtained as: \( \sigma (A) = \left\{ 1, \frac{3}{2} + \frac{\sqrt{7}}{2} i, \frac{3}{2} - \frac{\sqrt{7}}{2} i \right\} \).

Assume the eigenvalues of \( A \) having the following form:

\[
\lambda_0 = 1, \lambda_1 = \frac{3}{2} + \frac{\sqrt{7}}{2} i, \lambda_2 = \frac{3}{2} - \frac{\sqrt{7}}{2} i,
\]

(4.12)

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Then as in Example 4.1,
\[ f(A) = \alpha A + \beta A^2 + \eta_0 I \]  
(4.13)

Now, using Theorem 3.2 for supposing the scalar functions \( G(z) \) and \( H(z) \) which defined on the spectrum of square matrix \( A \) as the form: \( G(z) = z \) and \( H(z) = z^2 \) and using conditions then the constants \( \alpha, \beta \) and \( \eta_0 \) can be obtained as follows:
\[
\begin{align*}
\alpha &= (-1.6067250713848877', \quad \beta = (1.63032653156514' + 1.110223024625' \times 10^{-16} i), \quad \\
\eta_0 &= (2.6946803682787928' - 7.47924047217128' \times 10^{-17} i).
\end{align*}
\]
(4.14)

Then, using our technique which proposed in definition 3.1 and substitute from Eq. (4.14) in Eq. (4.12) we have:
\[
\begin{align*}
f(A) &= \begin{pmatrix}
-10.3243 - 8.519 \times 10^{-16} i & -3.30786 - 4.440 \times 10^{-16} i & -6.52131 - 4.440 \times 10^{-16} i \\
13.137 + 1.3322 \times 10^{-15} i & -0.542371 - 1.858 \times 10^{-16} i & 6.56851 + 6.661 \times 10^{-16} i \\
26.1324 + 1.998 \times 10^{-15} i & 3.33146 + 5.551 \times 10^{-16} i & 15.7845 + 1.035 \times 10^{-16} i
\end{pmatrix}
\]
(4.15)

Hence,
\[
f(A) = e^A = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
-2 & 2 & 0 & 0 & 0 \\
4 & 1 & 3 & 0 & 0 \\
0 & 0 & 0 & 1 & 2 \\
0 & 0 & 0 & -2 & 1
\end{pmatrix}
\]
\( \in \mathbb{C}^{5 \times 5} \), \( f(z) = \sqrt{z} \), then compute \( f(A) \).

**Example 4.4** Consider a square matrix \( A = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
-2 & 2 & 0 & 0 & 0 \\
4 & 1 & 3 & 0 & 0 \\
0 & 0 & 0 & 1 & 2 \\
0 & 0 & 0 & -2 & 1
\end{pmatrix} \in \mathbb{C}^{5 \times 5} \), then compute \( f(A) \).

The spectrum of \( A \) can be obtained as: \( \sigma(A) = \{1, 2, 3, 1 + 2i, 1 - 2i\} \).

Now, we suppose eigenvalues of \( A \) are ordered as: \( \lambda_0 = 1, \lambda_1 = 2, \lambda_2 = 3 \) (are distinct real eigenvalues) and \( \lambda_3 = 1 + 2i, \lambda_4 = 1 - 2i \) (are complex eigenvalues)

Since, \( \lambda_0 < \lambda_1 < \lambda_2 \) and \( \operatorname{Re} \lambda_3 \leq \operatorname{Re} \lambda_4, \quad n = 5 \). Then, applying our technique we have:
\[
f(A) = \alpha G(A) + \beta H(A) + \sum_{i=0}^{2} \eta_i A^i \]
(4.16)

Now, we using the conditions of our technique obtain the constants as:
\[
\begin{align*}
\alpha &= (0.03887163073825562' + 3.0799188767332846' \times 10^{-17} i), \\
\beta &= (-0.00420861471673508' - 1.734723475976807' \times 10^{-17} i), \\
\eta_0 &= (0.4076904657025189' + 2.20244609429313' \times 10^{-16} i), \\
\eta_1 &= (0.7338490934757743' + 3.39809894115261' \times 10^{-17} i), \\
\eta_2 &= (-0.17620257521981394' - 3.39809894115261' \times 10^{-17} i)
\end{align*}
\]
(4.16)

From Eq. (4.16) in Eq. (4.15), one can obtain:
\[
f(A) = \{ \{1, + 2.35497 \times 10^{-16} i, 0, 0, 0\}, \\
\{0, -0.828427 + 2.25152 \times 10^{-16} i, 1.41421 + 1.2292 \times 10^{-16} i, 0, 0, 0\}, \\
\{1.76364 - 1.00529 \times 10^{-16} i, 0.360823 - 2.87464 \times 10^{-16} i, 1.41421 + 1.22920 \times 10^{-16} i, 0, 0\}, \\
\{0, 0, 0, 1.27202 + 1.40608 \times 10^{-16} i, 0.786151 + 2.86773 \times 10^{-16} i\}, \\
\{0, 0, 0, -0.786151 - 2.86773 \times 10^{-16} i, 1.27202 + 1.40608 \times 10^{-16} i\}\}
\]
Remark: we notice that, the error appear in the imagine part and it is approximately equal to \((4.70993 \times 10^{-16}i)\). This implies that \((\sqrt{A})^2 \cong A\). Therefore, our proposed techniques in definition 3.1 can be used practically for approximating matrix functions of square matrices of higher order. Also this technique gives high accuracy for computing the square root of matrix \(A\).

Example 4.5 Consider a square matrix \(A = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -2 & 2 & 0 & 0 & 0 \\ 4 & 1 & 3 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & -2 & 1 \end{pmatrix} \in \mathbb{C}^{5 \times 5}, \ f(z) = e^z\). Then compute \(f(A)\).

Similarly to Example 4.4, the spectrum of \(A\) can be obtained as: \(\sigma(A) = \{1, 2, 3, 1 + 2i, 1 - 2i\}\).

As in Example 4.4 then, we have:

\[
 f(A) = \alpha A^3 + \beta A^4 + \eta_0 I + \eta_1 A + \eta_2 A^2
\]

Using conditions in our technique then, the constants \(\alpha, \beta, \eta_0, \eta_1\) and \(\eta_2\) can be obtained as in the following form:

\[
\begin{align*}
\alpha &= (-0.4848409330854552 - 1.3055465266988748 \times 10^{-16} \text{i}), \\
\beta &= (0.19586976187370028 + 5.551115123125783 \times 10^{-17} \text{i}), \\
\eta_0 &= (1.9309482828323714 - 2.220446049250313 \times 10^{-16} \text{i}), \\
\eta_1 &= (-0.9488501117245017 + 1.211450527097903 \times 10^{-16} \text{i}), \\
\eta_2 &= (2.02515482856293 - 1.2114505270979007 \times 10^{-16} \text{i})
\end{align*}
\]

Hence, substitute from Eq. (4.18) in Eq. (4.17) we have the matrix function \(f(A)\) as follows:

\[
 f(A) = e^A = \begin{Bmatrix}
 2.71828 - 2.97088 \times 10^{-16} \text{i}, 0, 0, 0, 0, \\
 -9.34155 + 6.47011 \times 10^{-16} \text{i}, 7.38906 - 6.20594 \times 10^{-16} \text{i}, 0, 0, 0, \\
 12.8216 - 1.63 \times 10^{-15} \text{i}, 7.60151 - 1.53 \times 10^{-16} \text{i}, 7.38906 - 6.20 \times 10^{-16} \text{i}, 0, 0, 0, \\
 0, 0, 0, -1.1312 + 1.31006 \times 10^{-15} \text{i}, 2.47173 - 1.31345 \times 10^{-15} \text{i}, \\
 0, 0, 0, -2.47173 + 1.31345 \times 10^{-15} \text{i}, -1.1312 + 1.31006 \times 10^{-15} \text{i}
\end{Bmatrix}
\]

This implies that we can use our technique for computing the exponential of square matrices of higher order having mixed eigenvalues because the error is very small as it is obvious in the results and we can ignore these errors in the imaginary part.

Remarks:

1. In all the examples of this paper we used MATHEMATICA 6 program for solving linear system of equations and other computations through solving these examples.

2. In all our examples we use polar coordinates to compute functions of complex eigenvalues and also different methods are used for solving the linear system of equations when we find constants of our problem.

3. We concentrate in this paper on square matrices having odd positive order because this types of matrices if it having complex eigenvalues must contain also real eigenvalues (mixed).

5 Concluding remarks

Computing matrix functions \(f(A)\) of \(n\)-by-\(n\) matrix \(A\) is a frequently occurring problem in control theory and other applications. In this paper, we presented a new technique for computing matrix functions \(f(A)\) of square matrices which has mixed eigenvalues, using numerical hybrid method. The proposed method is tested on several problems especially for square root and exponential of square matrices. The obtained results show that the new approach is efficient and practically in application. Also, these results illustrate the applicability of our technique and show that this technique gives high accuracy for approximating matrix functions \(f(A)\) for square matrices having mixed eigenvalues. This method can be used for solving some important problems in control theory.
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References


