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MATRIX FUNCTIONS APPROXIMATION FOR SQUARE MATRICES USING NEWTON'S INTERPOLATION

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Abstract: In this paper, we propose different formulas to approximating matrix functions for square matrices having (mixed or pure complex) eigenvalues. The suggested formulas are deduced from Newton's divided differences which defined for square matrices having real eigenvalues where we generalize it in our proposal cases. The theoretical analysis of these techniques is then discussed. Numerical examples are presented to illustrate the applicability and the accuracy of the obtained analytical results.

Keywords: Matrix function, Newton's divided differences, Polar coordinate, mixed eigenvalues, pure complex eigenvalues, a square matrix, square root of matrix,mixed interpolation.

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1. Introduction

Numerical methods for computing matrix functions having real eigenvalues have developed rapidly in the past three decades [4-6]. They have been applied successfully to numerical simulations in many fields [1, 2,5]. 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[6].As a result there have been distinct definitions of a matrix functions by Sylvester,Cauchy integral definition, Jordan canonical form and M. Dehghan, M. Hajarian (for more details see [2, 5, 6]).

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In this paper, we will discuss approximating matrix functions for square matrices having (mixed or pure complex) eigenvalues by using Newton's divided differences, and we will propose a new formula in each case for approximating these functions with some important examples to illustrate the applicability of suggested techniques.

This paper is organized as follows. In section 2, we give some important definitions for approximating matrix function$f(A)$. In section 3, we give our new formulas for approximating matrix function $f(A)$ which having (pure complex and mixed) eigenvalues, and we show that how we deduce the new formulas. In section 4, we illustrate the accuracy of our formulas by considering different numerical examples. Finally a brief conclusion ends of this paper.

2. Preliminaries

In this section, we introduce some definitions, methods and Corollaryfor computing matrix functionswhich will be used to implement our new approach. The following definitions are the most generally useful ones.

Definition 2.1([2]). Sylvester, in 1883, proposed the following definition of a matrix function corresponding to the scalar function $f\ (z)$ as:

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

where$A \in \mathbb{C}^{n+1 \times n+1}$is a square matrix with distinct characteristic roots$\lambda_0, \lambda_1, \cdots, \lambda_n$(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.

Definition 2.2([6]). Cauchy integral form of matrix functions.Let A $\in \mathbb{C}^{n \times n}$ be square matrix with eigenvalues $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ then, the matrix function $f(A)$ defined by:

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

whereΓ consists of a finite number of simple closed curves Γ_k with interiors Ω_k such that:

(a) $f(z)$is analytic on Γ_k and on Ω_k.

(b) Each λ_i is contained in someΩ_k.

Definition 2.3([5]). Jordan canonical form and matrix functions.It is a standard result that any matrix $A \in \mathbb{C}^{n\times n}$ can be expressed in the Jordan canonical form:

$$Z^{-1}AZ = J = diag(J_1, J_2, \cdots, J_p), \tag{2.3}$$

$$J_k = J_k(\lambda_k) = \begin{pmatrix} \lambda_k & 1 & 0 & 0 \\ 0 & \lambda_k & \ddots & 0 \\ 0 & 0 & \ddots & 1 \\ 0 & 0 & 0 & \lambda_k \end{pmatrix} \in \mathbb{C}^{m_k\times m_k}, \tag{2.4}$$

where$Z$ is nonsingular and $m_1 + m_2 + \cdots + m_p = n$. The Jordan matrix J is unique up to the ordering of the blokes J_i, but the transforming matrix Z is not unique.

Definition 2.4([5]). Matrix functions via Jordan canonical form.Let f be defined on the spectrum of $A \in \mathbb{C}^{n\times n}$ and let A have the Jordan canonical forms (2.3) and (2.4). Then,

$$f(A) = Zf(J)Z^{-1} = Z\, diag(f(J_k))Z^{-1}, \tag{2.5}$$

where

$$f(J_k) = \begin{pmatrix} f(\lambda_k) & \acute{f}(\lambda_k) & \cdots & \dfrac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ 0 & f(\lambda_k) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \acute{f}(\lambda_k) \\ 0 & 0 & \cdots & f(\lambda_k) \end{pmatrix} \tag{2.6}$$

Now, we explain how(2.6)can be obtained from Taylor series considerations. In (2.4) write $J_k = \lambda_k I + N_k \in \mathbb{C}^{m_k\times m_k}$, where N_k is zero except for a superdiagonal of 1s. Note that for $m_k = 3$ we have

$$N_k = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad N_k^2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad N_k^3 = 0.$$

In general, powering N_k causes the superdiagonal of 1s to move a diagonal at a time towards the top right-hand corner, until at the m_kth power it disappears: $N_k^{m_k} = 0$; so N_k is nilpotent. Assume that f has a convergent Taylor series expansion

$$f(t) = f(\lambda_k) + \acute{f}(\lambda_k)(t-\lambda_k) + \cdots + \frac{f^{(j)}(\lambda_k)(t-\lambda_k)^j}{j!} + \cdots .$$

On substituting $J_k \in \mathbb{C}^{m_k\times m_k}$ for t we obtain the finite series as:

(2.7) $$f(J_k) = f(\lambda_k)I + \acute{f}(\lambda_k)N_k + \cdots + \frac{f^{(m_k-1)}(\lambda_k)N_k^{m_k-1}}{(m_k-1)!}.$$

Since, all powers of N_k from the $m_k - th$ onwards are zero. This expression is easily seen to agree with (2.6).

Definition 2.5 ([2]). M. Dehghan and M. Hajarian, definition for matrix functions. Let A be an $(n+1)$-by- $(n+1)$ real matrix with distinct real eigenvalues, $\sigma(A) = \{\lambda_0, \lambda_1, \cdots, \lambda_n\}$ where $\lambda_0 < \lambda_1 < \cdots < \lambda_n$ and $f: \mathbb{C} \to \mathbb{C}$ be defined on the spectrum of A $(\sigma(A))$. Now M. Dehghan and M. Hajarian defined $f(A)$ as follows:

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

in which

(2.9) $$\begin{cases} K[\lambda_0] = f(\lambda_0), \\ K[\lambda_0, \lambda_1] = \dfrac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}, \\ K[\lambda_i, \lambda_{i+1}, \cdots, \lambda_{i+k}] = \dfrac{f[\lambda_{i+1}, \cdots, \lambda_{i+k}] - f[\lambda_i, \cdots, \lambda_{i+k-1}]}{\lambda_{i+k} - \lambda_i}. \end{cases}$$

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

Definition 2.6 ([2]). M.Dehghan and M.Hajarian definition for matrix functions. Let A be an $(n+1)$ -by- $(n+1)$ real matrix where its eigenvalues are not necessarily distinct, $\sigma(A) = \{\lambda_0, \lambda_1, \cdots, \lambda_n\}$ where $\lambda_0 \le \lambda_1 \le \cdots \le \lambda_n$, and $f: \mathbb{C} \to \mathbb{C}$ be defined on the spectrum of $A(\sigma(A))$ and $f(z)$ be a scalar analytic defined function at $z = \lambda_i$ for $i = 0, 1, \dots, n$. Now they defined matrix function $f(A)$ as follows:

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

in which

(2.11) $$\begin{cases} K[\lambda_0, \lambda_1] = \dfrac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}, & \\ K[\lambda_i, \lambda_{i+1}, \dots, \lambda_{i+k}] = \dfrac{f^{(k)}(\lambda_i)}{k!}, & \text{if } \lambda_i = \lambda_{i+k} \\ K[\lambda_i, \lambda_{i+1}, \dots, \lambda_{i+k}] = \dfrac{f[\lambda_{i+1}, \dots, \lambda_{i+k}] - f[\lambda_i, \dots, \lambda_{i+k-1}]}{(\lambda_{i+k} - \lambda_i)}, & otherwise. \end{cases}$$

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

(2.12) $$f(A) = f(\lambda)I + f'(\lambda)(A - \lambda I) + \frac{f''(\lambda)}{2!}(A - \lambda I)^2 + \cdots + \frac{f^{(n)}(\lambda)}{n!}(A - \lambda I)^n.$$

Definition 2.7 ([2]). Interpolation formula.The polynomial interpolation of degree n for a function f whose values are known at $n+1$ distinct points, $x_0, x_1, \cdots, x_n$, may be expressed in Newtonian form as

$$P_n(x) = f(x_0) + (x - x_0)f[x_1, x_0] + \cdots + (x - x_0)\cdots(x - x_{n-1})f[x_n, \cdots, x_0] \tag{2.13}$$

We will use this definition in case of a square matrix $A \in \mathbb{C}^{n\times n}$ which having eigenvalues λ_i , $i = 0,1,2, \dots, n-1$and aother forms of eigenvaluues.

Corollary 2.1 (**[7]).**Let $A \in \mathbb{C}^{n\times n}$ be a block matrix as in the form:

$$\mathrm{A} = \begin{pmatrix} \mathrm{A}_1 & 0 & 0 & 0 & 0 \\ 0 & \mathrm{A}_2 & 0 & 0 & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \mathrm{A}_\mathrm{k} \end{pmatrix} \text{then, } f(\mathrm{A}) = \begin{pmatrix} f(\mathrm{A}_1) & 0 & 0 & 0 & 0 \\ 0 & f(\mathrm{A}_2) & 0 & 0 & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \ddots & \cdots \\ \cdots & \cdots & \cdots & \cdots & f(\mathrm{A}_\mathrm{k}) \end{pmatrix} \tag{2.14}$$

where each A_i, $i = 1,2, \cdots,$ kis a square matrix of order less than the order of A (For more details for corollary 2.1, see [7]).

3. Main results

For the well known Newton's divided difference formula and Hermite interpolation for the polynomial interpolation as in definition (2.7).We extend and generalize this definition in case of a square matrix $A(A \in \mathbb{C}^{n\times n})$ having (pure complex or mixed) eigenvalues and other forms of eigenvalues.Since, Newton’s divided differences formula for any square matrix $A \in \mathbb{C}^{n\times n}$ having distinct real eigenvalues is given by:

$$\begin{aligned} f(A) = {} & f(\lambda_0)I + f[\lambda_0, \lambda_1](A - \lambda_0 I) + f[\lambda_0, \lambda_1, \lambda_2](A - \lambda_0 I)(A - \lambda_1 I) + \cdots \\ & + f[\lambda_0, \lambda_1, \lambda_2, \cdots, \lambda_{n-1}](A - \lambda_0 I)(A - \lambda_1 I)\cdots(A - \lambda_{n-2} I) \end{aligned} \tag{3.1}$$

where$\lambda_0 < \lambda_1 < \cdots < \lambda_{n-1}$are distinct real eigenvalues and

$$\begin{cases} f[\lambda_0, \lambda_1] = \dfrac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}, \\ f[\lambda_i, \lambda_{i+1}, \cdots, \lambda_{i+k}] = \dfrac{f[\lambda_{i+1}, \cdots, \lambda_{i+k}] - f[\lambda_i, \cdots, \lambda_{i+k-1}]}{\lambda_{i+k} - \lambda_i}, \\ i = 0,1, \cdots, n-1. \end{cases} \tag{3.2}$$

are Newton’s divided differences (for more details see M. Dehghan and M. Hajarian, 2009, ref.[2]).

The previous definition will be investigated for computing matrix functions for square matrices having (mixed or pure complex) eigenvalues. We illustrate the changes which occurred on definition of matrix functions as in Eq. (3.1) with aid Eq. (3.2), by giving brief formulas.
Next, we consider different stages (sizes) for our square matrix($A \in \mathbb{C}^{n\times n}$):

Study matrix functions for square matrices as the following:

Stage 1. Let$A \in \mathbb{C}^{2\times 2}$ be a square matrix, then there are two possible cases for its eigenvalues

Case 1.a. If A having two distinct real eigenvalues λ_0, λ_1 then

(3.3)$f(A) = f(\lambda_0) + f[\lambda_0, \lambda_1](A - \lambda_0 I)$(Discussed previously [2])

Case 1.b. If Ahaving one complex eigenvalue $\lambda_0$with its complex conjugate$\bar{\lambda}_0$, then, set:
$\lambda_0 = \alpha_0 + i\beta_0,\ \bar{\lambda}_0 = \alpha_0 - i\beta_0,\ \alpha_0, \beta_0 \in \mathbb{R}$and $\beta_0 \neq 0$. Then, we introduce the following suggested formula:

$$\begin{aligned} f(A) &= f(\lambda_0)I + f\left[\lambda_0, \bar{\lambda}_0\right](A - \lambda_0 I) = f(\lambda_0)I + \frac{f\left(\bar{\lambda}_0\right) - f(\lambda_0)}{\bar{\lambda}_0 - \lambda_0}(A - \lambda_0 I) \\ &= f(\lambda_0)I + \frac{f\left(\bar{\lambda}_0\right) - f(\lambda_0)}{-2i\beta_0}(A - \lambda_0 I) = g_0 I + \frac{g_0 - \bar{g}_0}{2i\beta_0}(A - \lambda_0 I) \\ &= g_0 I + H_{00}F_0 \end{aligned}$$

Hence, we have the first formula

Formula I

(3.4) $$f(A) = g_0 I + H_{00}F_0$$

where

(3.5) $$g_0 = f(\lambda_0),\ \overline{g}_0 = f\left(\bar{\lambda}_0\right),\ H_{00} = \frac{g_0 - \bar{g}_0}{2i\beta_0}\ ,\ F_0 = (A - \lambda_0 I).$$

Stage 2. Let$A \in \mathbb{C}^{3\times 3}$be a square matrix, then there are two cases for its eigenvalue

Case 2.a. If Ahaving three distinct real eigenvalues, $\lambda_0, \lambda_1, \lambda_2$such that $\lambda_0 < \lambda_1 < \lambda_2$then,

(3.6)$f(A) = f(\lambda_0)I + f[\lambda_0, \lambda_1](A - \lambda_0 I) + f[\lambda_0, \lambda_1, \lambda_2](A - \lambda_0 I)(A - \lambda_1 I)$ (Discussed in previously [2])

Case 2.b. If A having mixed eigenvalues (one real λ_0 and another complex $\lambda_1$with its complex conjugate $\overline{\lambda}_1$) then, a formula for computing matrix functions in this case will be suggested as follows:

First, suppose eigenvalues of A having the forms:

$\lambda_0 = \alpha_0,\quad \lambda_1 = \alpha_1 + i\beta_1,\quad \bar{\lambda}_1 = \alpha_1 - i\beta_1\quad , \alpha_1, \beta_1 \in \mathbb{R}and\beta_1 \neq 0$.

Then, the suggested matrix functions having the form:

(3.7) $$f(A) = f(\lambda_0)I + f[\lambda_0,\lambda_1](A-\lambda_0 I) + f[\lambda_0,\lambda_1,\bar{\lambda}_1](A-\lambda_0 I)(A-\lambda_1 I)$$

$$= f(\lambda_0)I + \frac{f(\lambda_1)-f(\lambda_0)}{\lambda_1-\lambda_0}(A-\lambda_0 I) + \frac{f[\lambda_1,\bar{\lambda}_1]-f[\lambda_0,\lambda_1]}{\bar{\lambda}_1-\lambda_0}(A-\lambda_0 I)(A-\lambda_1 I)$$

$$= g_0 I + \frac{g_1-g_0}{(\alpha_1-\alpha_0)+i\beta_0}F_0 + \frac{1}{(\alpha_1-\alpha_0)-i\beta_0}\{\frac{f(\bar{\lambda}_1)-f(\lambda_1)}{\bar{\lambda}_1-\lambda_1} - \frac{g_1-g_0}{(\alpha_1-\alpha_0)+i\beta_0}\}F_0F_1$$

$$= g_0 I + \frac{g_1-g_0}{\gamma_{10}}F_0 + \frac{1}{\bar{\gamma}_{10}}\left\{\frac{\bar{g}_1-g_1}{-2i\beta_1} - \frac{g_1-g_0}{\gamma_{10}}\right\}F_0F_1 = g_0 I + H_{10}F_0 + \frac{1}{\bar{\gamma}_{10}}\{H_{11}-H_{10}\}F_0F_1$$

Hence, formula (3.7) can be rewritten as the form:

Formula 2.

(3.8) $$f(A) = g_0\mathrm{I} + \mathrm{H}_{10}\mathrm{F}_0 + \frac{1}{\bar{\gamma}_{10}}\{H_{11}-\mathrm{H}_{10}\}\mathrm{F}_0\mathrm{F}_1$$

where: $g_k = f(\lambda_k), \bar{g}_k = f(\bar{\lambda}_k)$, $F_k = (A-\lambda_k I)$, $k = 0,1$, $H_{10} = \frac{g_1-g_0}{\gamma_{10}}$,

(3.9) $H_{11} = \frac{g_1-\bar{g}_1}{2i\beta_1}$, $\gamma_{10} = (\alpha_1-\alpha_0)+i\beta_0$ with its complex conjugate $\bar{\gamma}_{10}$

Stage 3. Let $A \in \mathbb{C}^{4\times 4}$ be a square matrix then, there are three possible cases of its eigenvalues to be discussed as follows:

Case 3.a. If A having four distinct real eigenvalues of forms $\lambda_0,\lambda_1,\lambda_2,\lambda_3$ such that $\lambda_0 < \lambda_1 < \lambda_2 < \lambda_3$ then, the suggested matrix functions having the form:

$$f(A) = f(\lambda_0)I + f[\lambda_0,\lambda_1](A-\lambda_0 I) + f[\lambda_0,\lambda_1,\lambda_2](A-\lambda_0 I)(A-\lambda_1 I) + f[\lambda_0,\lambda_1,\lambda_2,\lambda_3](A-\lambda_0 I)(A-\lambda_1 I)(A-\lambda_2 I)$$

(3.10)(discussed previously, see ref. [2])

Case 3.b. If A having mixed eigenvalues (two real and one complex with its complex conjugate) then, a formula to compute f(A) will be deduced as follows: First, assume eigenvalues of A having the forms:

$\lambda_0 = \alpha_0$, $\lambda_1 = \alpha_1$, (real distinct eigenvalues) $\lambda_2 = \alpha_2 + i\beta_2$, $\bar{\lambda}_2 = \alpha_2 - i\beta_2$ (complex eigenvalues) and $\alpha_k, \beta_2 \in \mathbb{R}$ and $\beta_2 \neq 0$ for $k = 0,1,2$.

Then, our suggested formula for computing matrix functions can be written as follows:

(3.11) $$f(A) = f(\lambda_0)I + f[\lambda_0,\lambda_1](A-\lambda_0 I) + f[\lambda_0,\lambda_1,\lambda_2](A-\lambda_0 I)(A-\lambda_1 I) + f[\lambda_0,\lambda_1,\lambda_2,\bar{\lambda}_2](A-\lambda_0 I)(A-\lambda_1 I)(A-\lambda_2 I)$$

$$= f(\lambda_0)I + \frac{f(\lambda_1) - f(\lambda_0)}{\lambda_1 - \lambda_0}(A - \lambda_0 I) + \frac{f[\lambda_1, \lambda_2] - f[\lambda_0, \lambda_1]}{\lambda_2 - \lambda_1}(A - \lambda_0 I)(A - \lambda_1 I)$$

$$+ \frac{f[\lambda_1, \lambda_2, \bar{\lambda}_2] - f[\lambda_0, \lambda_1, \lambda_2]}{\bar{\lambda}_2 - \lambda_0}(A - \lambda_0 I)(A - \lambda_1 I)(A - \lambda_2 I) \qquad (3.12)$$

(3.13)Set: $g_k = f(\lambda_k), \bar{g}_k = f(\bar{\lambda}_k)$, $F_k = (A - \lambda_k I)$ $k = 0,1,2.$

Then, use Eq. (3.13) in formula (3.12), we get $f(A)$ as:

$$f(A) = g_0 I + \frac{g_1 - g_0}{\alpha_1 - \alpha_0}F_0 + \frac{1}{(\alpha_2 - \alpha_0) + i\beta_2}\left\{\frac{f(\lambda_2) - f(\lambda_1)}{\lambda_2 - \lambda_1} - \frac{g_1 - g_0}{\alpha_1 - \alpha_0}\right\}F_0F_1$$

$$+ \frac{1}{(\alpha_2 - \alpha_0) - i\beta_2}\left\{\frac{f[\lambda_2, \bar{\lambda}_2] - f[\lambda_1, \lambda_2]}{\bar{\lambda}_2 - \lambda_1} - \frac{f[\lambda_1, \lambda_2] - f[\lambda_0, \lambda_1]}{\lambda_2 - \lambda_0}\right\}F_0F_1F_2 \qquad (3.14)$$

(3.15)Now, suppose: $\gamma_{lj} = \lambda_l - \lambda_j$, $l = 1,2$, $j = 0,1$ and $l \neq j$ with their complex conjugates $\bar{\gamma}_{lj}$

Now, from Eq. (3.15) in formula (3.14) we have:

$$f(A) = g_0 I + \frac{g_1 - g_0}{\gamma_{10}}F_0 + \frac{1}{\gamma_{20}}\{\frac{g_2 - g_1}{(\alpha_2 - \alpha_1) + i\beta_2} - \frac{g_1 - g_0}{\gamma_{10}}\}F_0F_1$$

$$+ \frac{1}{\bar{\gamma}_{20}}\left\{\frac{1}{(\alpha_2 - \alpha_1) - i\beta_2}\left\{\frac{f(\bar{\lambda}_2) - f(\lambda_2)}{\bar{\lambda}_2 - \lambda_2} - \frac{f(\lambda_2) - f(\lambda_1)}{\lambda_2 - \lambda_1}\right\} - \frac{1}{\gamma_{20}}\left\{\frac{g_2 - g_1}{\gamma_{21}} - \frac{g_1 - g_0}{\gamma_{10}}\right\}\right\}F_0F_1F_2$$

$$= g_0 I + \frac{g_1 - g_0}{\gamma_{10}}F_0 + \frac{1}{\gamma_{20}}\left\{\frac{g_2 - g_1}{\gamma_{21}} - \frac{g_1 - g_0}{\gamma_{10}}\right\}F_0F_1 \qquad (3.16)$$

$$+ \frac{1}{\bar{\gamma}_{20}}\left\{\frac{1}{\bar{\gamma}_{21}}\left\{\frac{\bar{g}_2 - g_2}{-2i\beta_2} - \frac{g_2 - g_1}{\gamma_{10}}\right\} - \frac{1}{\gamma_{20}}\left\{\frac{g_2 - g_1}{\gamma_{21}} - \frac{g_1 - g_0}{\gamma_{10}}\right\}\right\}F_0F_1F_2$$

Also, suppose:

$$(3.17)\quad H_{10} = \frac{g_1 - g_0}{\gamma_{10}}, \qquad H_{21} = \frac{g_2 - g_1}{\gamma_{21}}, \quad H_{22} = \frac{g_2 - \bar{g}_2}{2i\beta_2}$$

then from Eq. (3.17) in formula (3.16) we have:

$$f(A) = g_0 I + H_{10}F_0 + \frac{1}{\gamma_{20}}\{H_{21} - H_{10}\}F_0F_1 + \frac{1}{\bar{\gamma}_{20}}\left\{\frac{1}{\bar{\gamma}_{21}}\{H_{22} - H_{21}\} - \frac{1}{\gamma_{20}}\{H_{21} - H_{10}\}\right\}F_0F_1F_2$$

Hence, formula (3.11) can be rewritten as:

Formula 3.

$$f(A) = g_0 I + H_{10}F_0 + \frac{1}{\gamma_{20}}\{H_{21} - H_{10}\}F_0F_1 + \frac{1}{\bar{\gamma}_{20}}\left\{\frac{1}{\bar{\gamma}_{21}}\{H_{22} - H_{21}\} - \frac{1}{\gamma_{20}}\{H_{21} - H_{10}\}\right\}F_0F_1F_2 \qquad (3.18)$$

where: $g_k = f(\lambda_k), \bar{g}_k = f(\bar{\lambda}_k)$, $F_k = (A - \lambda_k I)$, $k = 0,1,2$, $H_{10} = \frac{g_1 - g_0}{\gamma_{10}}$, $H_{21} = \frac{g_2 - g_1}{\gamma_{21}}$, $H_{22} = \frac{g_2 - \bar{g}_2}{2i\beta_2}$ and(3.19) $\gamma_{lj} = \lambda_l - \lambda_j$, $l = 1,2$, $j = 0,1$ and $l \neq j$ with their complex conjugates $\bar{\gamma}_{lj}$.

Case 3.c. If A having only pure complex eigenvalues (two complex eigenvalues $\lambda_0, \lambda_1$with their complex conjugates$\bar{\lambda}_0, \bar{\lambda}_1$ respectively) then, we will deducea formula to compute $f(A)$ as follows:

First, we assume eigenvalues of a matrix A having the forms:

(3.20) $$\lambda_0 = \alpha_0 + i\beta_0, \quad \bar{\lambda}_0 = \alpha_0 - i\beta_0, \quad \lambda_1 = \alpha_1 + i\beta_1, \quad \bar{\lambda}_1 = \alpha_1 - i\beta_1$$

where $\alpha_r,\beta_r \in \mathbb{R}$, $\beta_r \neq 0$ and $r = 0,1$. Then, our suggested formula can be written as in the following form:

(3.21) $$f(A) = f(\lambda_0)I + f[\lambda_0, \bar{\lambda}_0](A - \lambda_0 I) + f[\lambda_0, \bar{\lambda}_0, \lambda_1](A - \lambda_0 I)(A - \bar{\lambda}_0 I) + f[\lambda_0, \bar{\lambda}_0, \lambda_1, \bar{\lambda}_1](A - \lambda_0 I)(A - \bar{\lambda}_0 I)(A - \lambda_1 I)$$

$$= f(\lambda_0)I + \frac{f(\bar{\lambda}_0) - f(\lambda_0)}{\bar{\lambda}_0 - \lambda_0}(A - \lambda_0 I) + \frac{f[\bar{\lambda}_0, \lambda_1] - f[\lambda_0, \bar{\lambda}_0]}{\lambda_1 - \lambda_0}(A - \lambda_0 I)(A - \bar{\lambda}_0 I)$$

(3.22) $$+ \frac{f[\bar{\lambda}_0, \lambda_1, \bar{\lambda}_1] - f[\lambda_0, \bar{\lambda}_0, \lambda_1]}{\bar{\lambda}_1 - \lambda_0}(A - \lambda_0 I)(A - \bar{\lambda}_0 I)(A - \lambda_1 I)$$

(3.23)Now, Suppose:$g_k = f(\lambda_k), \bar{g}_k = f(\bar{\lambda}_k)$, $F_k = (A - \lambda_k I), \bar{F}_k = (A - \bar{\lambda}_k I)$, $k = 0,1$

Then, from Eq. (3.23) in formula (3.22) we have$f(A)$ as the form:

$$f(A) = g_0 I + \frac{\bar{g}_0 - g_0}{-2i\beta_0}F_0 + \frac{1}{(\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)}\left\{\frac{f(\lambda_1) - f(\bar{\lambda}_0)}{\lambda_1 - \bar{\lambda}_0} - \frac{f(\bar{\lambda}_0) - f(\lambda_0)}{\bar{\lambda}_0 - \lambda_0}\right\}F_0\bar{F}_0$$
$$+\left\{\frac{f[\bar{\lambda}_0, \lambda_1, \bar{\lambda}_1] - f[\lambda_0, \bar{\lambda}_0, \lambda_1]}{\bar{\lambda}_1 - \lambda_0}\right\}(A - \lambda_0 I)(A - \bar{\lambda}_0 I)(A - \lambda_1 I)$$

$$= g_0 I + \frac{g_0 - \bar{g}_0}{2i\beta_0}F_0 + \frac{1}{(\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)}\left\{\frac{g_1 - \bar{g}_0}{(\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\}F_0\bar{F}_0$$
$$+ \frac{1}{(\alpha_1 - \alpha_0) - i(\beta_1 + \beta_0)}\left\{\frac{1}{(\alpha_1 - \alpha_0) - i(\beta_1 - \beta_0)}\left\{\frac{f(\bar{\lambda}_1) - f(\lambda_1)}{\bar{\lambda}_1 - \lambda_1} - \frac{f(\lambda_1) - f(\bar{\lambda}_0)}{\lambda_1 - \bar{\lambda}_0}\right\}\right.$$
$$\left.- \frac{1}{(\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)}\left\{\frac{g_1 - \bar{g}_0}{(\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\}\right\}F_0\bar{F}_0F_1$$

$$= g_0 I + \frac{g_0 - \bar{g}_0}{2i\beta_0}F_0 + \frac{1}{(\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)}\left\{\frac{g_1 - \bar{g}_0}{(\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\}F_0\bar{F}_0$$
$$+ \frac{1}{(\alpha_1 - \alpha_0) - i(\beta_1 + \beta_0)}\left\{\frac{1}{(\alpha_1 - \alpha_0) - i(\beta_1 - \beta_0)}\left\{\frac{\bar{g}_1 - g_1}{-2i\beta_1} - \frac{g_1 - \bar{g}_0}{(\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)}\right\}\right.$$

(3.24) $$\left.- \frac{1}{(\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)}\left\{\frac{g_1 - \bar{g}_0}{(\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\}\right\}F_0\bar{F}_0F_1$$

Also, set:

(3.25) $\begin{cases}\gamma_{10} = (\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)\\ \mu_{10} = (\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)\end{cases}$ with their complex conjugates $\overline{\gamma}_{10}, \bar{\mu}_{10}$ respectively.

Now, from Eq. (3.25) in formula (3.24) we have:

$$f(A) = g_0 I + \frac{g_0 - \bar{g}_0}{2i\beta_0} F_0 + \frac{1}{\gamma_{10}}\left\{\frac{g_1 - \bar{g}_0}{\mu_{10}} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\} F_0 \bar{F}_0$$

(3.26) $$+ \frac{1}{\bar{\mu}_{10}}\left\{\frac{1}{\bar{\gamma}_{10}}\left\{\frac{g_1 - \bar{g}_1}{2\mathrm{i}\beta_1} - \frac{g_1 - \bar{g}_0}{\mu_{10}}\right\} - \frac{1}{\gamma_{10}}\left\{\frac{g_1 - \bar{g}_0}{\mu_{10}} - \frac{g_0 - \bar{g}_0}{2i\beta_0}\right\}\right\} F_0 \bar{F}_0 F_1$$

(3.27) Suppose that: $H_{00} = \frac{g_0 - \bar{g}_0}{2i\beta_0}$, $H_{10} = \frac{g_1 - \bar{g}_0}{\mu_{10}}$, $H_{11} = \frac{g_1 - \bar{g}_1}{2i\beta_1}$

Then, from Eq. (3.27) in formula (3.26) we can rewrite formula (3.21) in the following form:

Formula 4.

(3.28) $$f(A) = g_0 I + H_{00} F_0 + \frac{1}{\gamma_{10}}[H_{10} - H_{00}] F_0 \bar{F}_0 + \frac{1}{\bar{\mu}_{10}}\left\{\frac{1}{\bar{\gamma}_{10}}[H_{11} - H_{10}] - \frac{1}{\gamma_{10}}[H_{10} - H_{00}]\right\} F_0 \bar{F}_0 F_1$$

where:

(3.29) $g_k = f(\lambda_k), \bar{g}_k = f(\bar{\lambda}_k)$, $F_k = (A - \lambda_k I), \bar{F}_k = (A - \bar{\lambda}_k I)$, $k = 0,1$ and $H_{00} = \frac{g_0 - \bar{g}_0}{2i\beta_0}$, $H_{10} = \frac{g_1 - \bar{g}_0}{\mu_{10}}$, $H_{11} = \frac{g_1 - \bar{g}_1}{2i\beta_1}$,

$\gamma_{10} = (\alpha_1 - \alpha_0) + i(\beta_1 - \beta_0)$ with its complex conjugate $\bar{\gamma}_{10}$ and $\mu_{10} = (\alpha_1 - \alpha_0) + i(\beta_1 + \beta_0)$ with its complex conjugate $\bar{\mu}_{10}$.

Now, from the previous discussion, we can introduce some possible cases of the divided difference tables which help us in computing matrix functions of square matrices having (mixed or pure complex) eigenvalues as follows:

First: For a square matrix which having odd order eigenvalues (mixed eigen-values) we can discuss it as follows:

1- Let $A \in \mathbb{C}^{3\times3}$ having (one real eigenvalue λ_0 and another complex λ_1 with its complex conjugate $\overline{\lambda}_1$) then, we can obtain the table of divided differences in this case takes the form:

$$\begin{array}{cccc}
\lambda_0 & g_0 & & \\
 & & H_{10} & \\
\lambda_1 & g_1 & & W_{10} \\
 & & H_{11} & \\
\bar{\lambda}_1 & \bar{g}_1 & &
\end{array}$$

where: $g_i = f(\lambda_i)$, $H_{10} = \frac{g_1 - g_0}{\lambda_1 - \lambda_0}$, $H_{11} = \frac{g_1 - \bar{g}_1}{\lambda_1 - \bar{\lambda}_1}$, $W_{10} = \frac{H_{11} - H_{10}}{\bar{\lambda}_1 - \lambda_0}$, $\quad i = 0,1.$

Second: For a square matrix having even order eigenvalues (complex eigenvalues) we can discuss it as follows:

1- Let $A \in \mathbb{C}^{4\times 4}$ having pure complex eigenvalues (two complexes with theircomplex conjugates) then the table of divided differences takes the form:

$$
\begin{array}{ccccc}
\lambda_0 & g_0 & & & \\
 & & H_{00} & & \\
\bar{\lambda}_0 & \bar{g}_0 & & W_{00} & \\
 & & H_{10} & & L_{00} \\
\lambda_1 & g_1 & & W_{10} & \\
 & & H_{11} & & \\
\bar{\lambda}_1 & \bar{g}_1 & & &
\end{array}
$$

where: $H_{00} = \frac{g_0 - \bar{g}_0}{\lambda_0 - \bar{\lambda}_0}$, $H_{10} = \frac{g_1 - \bar{g}_0}{\lambda_1 - \bar{\lambda}_0}$, $W_{10} = \frac{H_{10} - H_{00}}{\lambda_1 - \lambda_0}$, $L_{00} = \frac{W_{10} - W_{00}}{\bar{\lambda}_1 - \lambda_0}$ and the reminder terms in the table can obtained by the same method as in thisrelations.

2- Let $A \in \mathbb{C}^{4\times 4}$ having mixed eigenvalues (two real eigenvalues and one complex with its complex conjugate) then the table of divided differences takes the form:

$$
\begin{array}{ccccc}
\lambda_0 & g_0 & & & \\
 & & H_{10} & & \\
\lambda_1 & g_1 & & W_{10} & \\
 & & H_{21} & & L_{10} \\
\lambda_2 & g_2 & & W_{21} & \\
 & & H_{22} & & \\
\bar{\lambda}_2 & \bar{g}_2 & & &
\end{array}
$$

where $H_{10} = \frac{g_1 - g_0}{\lambda_1 - \lambda_0}$, $H_{21} = \frac{g_2 - g_1}{\lambda_2 - \lambda_1}$, $W_{10} = \frac{H_{21} - H_{10}}{\lambda_2 - \lambda_0}$, $L_{10} = \frac{W_{21} - W_{10}}{\bar{\lambda}_2 - \lambda_0}$ and the reminder terms in the table can obtained by the same method of this relations.

Remark: If $A \in \mathbb{C}^{n\times n}$ be a square matrix having mixed or pure complex eigenvalues then, we can construct divided differences table by follow the same technique as in previous tables.

4. Numerical examples

In this section, we give several different numerical examples to support our theoretical results and to illustrate the applicability and the accuracy of the presented formulas for computing $f(A)$

where A is a square matrix having (mixed or pure complex) eigenvalues. Also, polar coordinate will be used for computing the functions of complex eigenvalues.

Example 4.1

Let$A = \begin{pmatrix} 1 & -2 \\ 2 & 1 \end{pmatrix}, f(z) = \sqrt{z}$then compute$f(A)$.

First, it is not difficult to have eigenvalues of A are of the form:

$$(4.1)\lambda_0 = 1 + 2i, \quad \bar{\lambda}_0 = 1 - 2i$$

Now, using **formula 1** as in Eq.$(3.4)$and Eq.$(3.5)$for computing $f(A)$.Then, we compute each term of **formula 1** as follows:

$g_0 = f(\lambda_0) = \sqrt{\lambda_0} = \sqrt{1+2i}$(using polar coordinates). Hence, we get

$g_0 = (1.272019649514069` + 0.7861513777574233` \, i) , \bar{g}_0 = (1.272019649514069` - 0.7861513777574233` \, i),$

(4.2) $H_{00} = \frac{2 \times 0.7861513777574233` \, i}{2i \times 2} = 0.39307568887871164`andF_0 = \begin{pmatrix} 1 & -2 \\ 2 & 1 \end{pmatrix} - (1+2i) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -2i & -2 \\ 2 & -2i \end{pmatrix}$

Now, substitute from Eq. (4.2) in **formula 1** get the result:

$$f(A) = (1.272019649514069` + 0.7861513777574233` \, i) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 0.39307568887871164` \begin{pmatrix} -2i & -2 \\ 2 & -2i \end{pmatrix}$$

(4.3) $$= \begin{pmatrix} 1.272019649514069` & -0.7861513777574233` \\ 0.7861513777574233` & 1.272019649514069` \end{pmatrix}$$

Notice that:$f(A) = \sqrt{A}, \left(f(A)\right)^2 = \sqrt{A} \cdot \sqrt{A} = A.$ So, we test our approximation as follows:

$$\sqrt{A} \cdot \sqrt{A} = \begin{pmatrix} 1.272019649514069` & -0.7861513777574233` \\ 0.7861513777574233` & 1.272019649514069` \end{pmatrix} . \begin{pmatrix} 1.272019649514069` & -0.7861513777574233` \\ 0.7861513777574233` & 1.272019649514069` \end{pmatrix}$$

(4.4) $$\cong \begin{pmatrix} 1 & -2 \\ 2 & 1 \end{pmatrix} = A$$

It is clear that: from Eq. (4.3) and Eq. (4.4) our formula 1 gives high accuracy to approximate matrix functions for a square matrix $A \in \mathbb{C}^{2\times 2}$ which having pure complex eigenvalues.

Example 4.2

Let $A = \begin{pmatrix} 1 & -2 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix}$, $f(z) = \sqrt{z}$then compute$f(A)$.

First, it is not difficult to obtain the eigenvalues of A as the form:

$$(4.5)\lambda_0 = 1 + 2i, \qquad \bar{\lambda}_0 = 1 - 2i, \lambda_1 = 3 + 4i, \bar{\lambda}_1 = 3 - 4i.$$

Formula 4 as in Eq. (3.28) and Eq. (3.29) can be applied practically for computing matrix function $f(A)$ in this case as follows:

Now, each term in **formula 4** can be computed as the following:

$$g_0 = (1.272019649514069` + 0.7861513777574233`\, i\,), \bar{g}_0$$
$$= (1.272019649514069` - 0.7861513777574233`\, i\,),$$

$g_1 = 2 + i, \bar{g}_1 = 2 - i$, $\gamma_{10} = 2 + 2i$, $\bar{\gamma}_{10} = 2 - 2i$, $\mu_{10} = 2 + 6i$ and $\bar{\mu}_{10} = 2 - 6i$

$$H_{00} = \frac{2 \times 0.7861513777574233`\, i}{2i \times 2} = 0.39307568887871164`$$

$$H_{10} = \frac{2 + i - 1.27 + 0.7861513777574233`\, i}{2 + 6i} = \frac{0.73 + 1.7861513777574233`\, i}{2 + 6i}$$
$$= (0.3044227066636135` - 0.02019243111212882`i)$$

$$H_{11} = \frac{2i}{2i \times 4} = \frac{1}{4} = 0.25$$

$$\frac{1}{\gamma_{10}}(H_{10} - H_{00}) = \frac{(-0.08865298221509815` - 0.02019243111212882`i)}{2 + 2i}$$
$$= -0.027211353331806742` + 0.017115137775742334\,`i$$

$$\frac{1}{\bar{\gamma}_{10}}(H_{11} - H_{10}) = \frac{0.25 - (0.3044227066636135` - 0.02019243111212882`i)}{2 - 2i}$$
$$= (-0.018653784443935575` - 0.008557568887871167`i)$$

$$\frac{1}{\bar{\mu}_{10}}\left[\frac{1}{\bar{\gamma}_{10}}(H_{11} - H_{10}) - \frac{1}{\gamma_{10}}(H_{10} - H_{00})\right] = \frac{(-0.01865` - 0.008557`i) + 0.027211` - 0.01711513\,`i}{2 - 6i}$$
$$= (0.001557649110754909` - 0.008163405999542022`i)$$

$$F_0 = \begin{pmatrix} 1 & -2 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix} - (1 + 2i)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -2i & -2 & 0 & 0 \\ 2 & -2i & 0 & 0 \\ 0 & 0 & 2 - 2i & -4 \\ 0 & 0 & 4 & 2 - 2i \end{pmatrix}$$

$$\bar{F}_0 = \begin{pmatrix} 2i & -2 & 0 & 0 \\ 2 & 2i & 0 & 0 \\ 0 & 0 & 2 + 2i & -4 \\ 0 & 0 & 4 & 2 + 2i \end{pmatrix}$$

$$F_0\bar{F}_0=\begin{pmatrix}-2i & -2 & 0 & 0\\ 2 & -2i & 0 & 0\\ 0 & 0 & 2-2i & -4\\ 0 & 0 & 4 & 2-2i\end{pmatrix}\begin{pmatrix}2i & -2 & 0 & 0\\ 2 & 2i & 0 & 0\\ 0 & 0 & 2+2i & -4\\ 0 & 0 & 4 & 2+2i\end{pmatrix}=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & -8 & -16\\ 0 & 0 & 16 & -8\end{pmatrix}$$

$$F_1=\begin{pmatrix}1 & -2 & 0 & 0\\ 2 & 1 & 0 & 0\\ 0 & 0 & 3 & -4\\ 0 & 0 & 4 & 3\end{pmatrix}-(3+4i)\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}=\begin{pmatrix}-2-4i & -2 & 0 & 0\\ 2 & -2-4i & 0 & 0\\ 0 & 0 & -4i & -4\\ 0 & 0 & 4 & -4i\end{pmatrix}$$

$$F_0\bar{F}_0F_1=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & -8 & -16\\ 0 & 0 & 16 & -8\end{pmatrix}\begin{pmatrix}-2-4i & -2 & 0 & 0\\ 2 & -2-4i & 0 & 0\\ 0 & 0 & -4i & -4\\ 0 & 0 & 4 & -4i\end{pmatrix}=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & -64+32i & 32+64i\\ 0 & 0 & -32-64i & -64+32i\end{pmatrix}$$

Now, substitute from the above calculation in **formula 4** we have:

$$f(A)=(1.272019649514069` + 0.7861513777574233`\, i\,)I+0.39307568887871164`F_0$$

$$+(-0.027211353331806742` + 0.017115137775742334`i\,)F_0\bar{F}_0$$

$$+(0.001557649110754909` - 0.008163405999542022`i)F_0\bar{F}_0F_1$$

$$=\begin{pmatrix}1.27202 & -0.786151 & 0 & 0\\ 0.786151 & 1.27202 & 0 & 0\\ 0 & 0 & 2 & -1.00006\\ 0 & 0 & 1.00006 & 2\end{pmatrix}$$

Hence, we have the matrix function $f(A)$ as the form:

$$f(A)=\sqrt{A}=\begin{pmatrix}1.27202 & -0.786151 & 0 & 0\\ 0.786151 & 1.27202 & 0 & 0\\ 0 & 0 & 2 & -1.00006\\ 0 & 0 & 1.00006 & 2\end{pmatrix} \tag{4.6}$$

Notice that:

$f(A)=\sqrt{A}\,,\big(f(A)\big)^2=\sqrt{A}\cdot\sqrt{A}=A$.Then, our approximation will be tested as follows:

$$\big(f(A)\big)^2$$

$$=\begin{pmatrix}1.27202 & -0.786151 & 0 & 0\\ 0.786151 & 1.27202 & 0 & 0\\ 0 & 0 & 2 & -1.00006\\ 0 & 0 & 1.00006 & 2\end{pmatrix}\begin{pmatrix}1.27202 & -0.786151 & 0 & 0\\ 0.786151 & 1.27202 & 0 & 0\\ 0 & 0 & 2 & -1.00006\\ 0 & 0 & 1.00006 & 2\end{pmatrix}$$

$$=\begin{pmatrix}1 & -2 & 0 & 0\\ 2 & 1 & 0 & 0\\ 0 & 0 & 2.99988 & -4.00024\\ 0 & 0 & 4.00024 & 2.99988\end{pmatrix}\cong\begin{pmatrix}1 & -2 & 0 & 0\\ 2 & 1 & 0 & 0\\ 0 & 0 & 3 & -4\\ 0 & 0 & 4 & 3\end{pmatrix}=A \tag{4.7}$$

Remark: the results in Eq. (4.6) and Eq. (4.7) illustrate the applicability of our investigated formula and showed that this formula gives high accuracy for computing matrix functions of square matrices $A \in \mathbb{C}^{4\times4}$ having pure complex eigenvalues. Also, this example can be solved by considering it block diagonal square matrix.

Example 4.3

Let $A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix}, f(z) = \sqrt{z}$then compute$f(A)$.

First, we can obtain eigenvalues of it by using $|A - \lambda I| = 0$

Hence, $\sigma(A) = \{1,4,3+4i, 3-4i\}$so that suppose:eigenvalues of A having the forms:

(4.8) $\lambda_0 = 1,\quad \lambda_1 = 4$(two real eigenvalues)$\lambda_2 = 3+4i,\ \bar{\lambda}_2 = 3-4i$(complex eigenvalue with its C. C.)

Since eigenvalues of a square matrix are mixed then, **formula 3** as in Eq. (3.18) and Eq. (3.19) can be applied practically for computing $f(A)$. Now, each term in **formula 3** can be computed as:

$g_0 = 1,\ g_1 = 2,\ and\ \ g_2 = 2+i, \bar{g}_2 = 2-i$ (computed using polar coordinates)

$\gamma_{10} = 3,\ \ \gamma_{20} = 2+4i,\ \bar{\gamma}_{20} = 2-4i,\ \gamma_{21} = -1+4i,\ \bar{\gamma}_{21} = -1-4i,$

$H_{10} = \frac{1}{3}, \qquad H_{21} = \frac{4-i}{17}, \qquad H_{22} = \frac{1}{4},$

$$\frac{1}{\gamma_{20}}(H_{21} - H_{10}) = \frac{1}{2+4i}\left(\frac{4-i}{17} - \frac{1}{3}\right) = -\frac{5+3i}{51(2+4i)} = \frac{-11+4i}{510} = -0.02157 + 0.00784i$$

$$\frac{1}{\bar{\gamma}_{21}}(H_{22} - H_{21}) = \frac{1}{-1-4i}\left(\frac{1}{4} - \frac{4-i}{17}\right) = \frac{-1}{1+4i}\left(\frac{1+4i}{68}\right) = \frac{-1}{68}$$

$$\frac{1}{\bar{\gamma}_{20}}\left[\frac{1}{\bar{\gamma}_{21}}(H_{22} - H_{21}) - \frac{1}{\gamma_{20}}(H_{21} - H_{10})\right] = \frac{1}{2-4i}\left[\frac{-1}{68} + 0.02157 - 0.00784i\right] = \frac{0.00686 - 0.00784i}{2-4i}$$

$$= \frac{0.04508 + 0.01176i}{20} = 0.00225 + 0.00059i$$

$$F_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & -4 \\ 0 & 0 & 4 & 2 \end{pmatrix},$$

$$F_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix} - 4\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -4 \\ 0 & 0 & 4 & -1 \end{pmatrix}$$

$$F_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 3 & -4 \\ 0 & 0 & 4 & 3 \end{pmatrix} - (3+4i)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} -2-4i & 0 & 0 & 0 \\ 0 & 1-4i & 0 & 0 \\ 0 & 0 & -4i & -4 \\ 0 & 0 & 4 & -4i \end{pmatrix}$$

$$F_0F_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & -4 \\ 0 & 0 & 4 & 2 \end{pmatrix}\begin{pmatrix} -3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -4 \\ 0 & 0 & 4 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -18 & -4 \\ 0 & 0 & 4 & -18 \end{pmatrix}$$

$$F_0F_1F_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -18 & -4 \\ 0 & 0 & 4 & -18 \end{pmatrix}\begin{pmatrix} -2-4i & 0 & 0 & 0 \\ 0 & 1-4i & 0 & 0 \\ 0 & 0 & -4i & -4 \\ 0 & 0 & 4 & -4i \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -16+72i & 72+16i \\ 0 & 0 & -72-16i & -16+72i \end{pmatrix}$$

Now, we substitute from the above calculation in **formula 3** (Eq. (3.18)) then, we get the matrix function $f(A)$ having the form:

$$\begin{aligned} f(A) &= I + \frac{1}{3}F_0 + (-0.02157 + 0.00784i)F_0F_1 + (0.00225 + 0.00059i)F_0F_1F_2 \\ &= I + \frac{1}{3}F_0 - 0.02157F_0F_1 + 0.00225F_0F_1F_2 + i(0.00784F_0F_1 + 0.00059F_0F_1F_2) \end{aligned}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2.01893 + 0.162i & -1.085053 + 0.036i \\ 0 & 0 & 1.085053 - 0.036i & 2.01893 + 0.162i \end{pmatrix} + i\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -0.15056 + 0.04248i & 0.01112 + 0.00944i \\ 0 & 0 & -0.01112 - 0.00944i & -0.15056 + 0.04248i \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1.97645 + 0.01i & -1.094493 + 0.04i \\ 0 & 0 & 1.094493 - 0.04i & 1.97645 + 0.01i \end{pmatrix} \cong \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1.97465 & -1.094493 \\ 0 & 0 & 1.094493 & 1.97465 \end{pmatrix}$$

Hence, the principle square root of a given matrix is:

$$f(A) = \sqrt{A} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1.97465 & -1.094493 \\ 0 & 0 & 1.094493 & 1.97465 \end{pmatrix} \tag{4.9}$$

Notice that: $f(A) = \sqrt{A}\,, \big(f(A)\big)^2 = \sqrt{A}\cdot\sqrt{A} \cong A$

It’s clear that: as obtained results in Eq. (4.9) andour formula gives height accuracy for computing matrix functions of square matrices $A \in \mathbb{C}^{4\times 4}$ which having mixed (two real and the other complex with its complex conjugate) eigenvalues.

Example 4.4

Let $A = \begin{pmatrix} 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 3 & -4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 & 4 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 3 & -4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 4 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 & 0 & 1 & 10 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 1 & 2 & 8 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 3 & 2 & 7 & 5 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & -4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 3 \end{pmatrix} \in \mathbb{C}^{11\times 11}$, $f(z) = \sqrt{z}$then compute$f(A)$.

This square matrix can be rewritten in the form of block diagonal matrix as:

$A = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}$where$A_1 = \begin{pmatrix} 1 & -2 \\ 2 & 1 \end{pmatrix}$, $A_2 = \begin{pmatrix} 1 & -2 & 3 & -4 \\ 2 & 1 & 4 & 3 \\ 0 & -2 & 3 & -4 \\ 0 & 1 & 4 & 3 \end{pmatrix}andA_3 = \begin{pmatrix} 1 & -2 & 0 & 1 & 10 \\ 4 & 1 & 2 & 8 & 6 \\ 2 & 3 & 2 & 7 & 5 \\ 0 & 0 & 0 & 3 & -4 \\ 0 & 0 & 0 & 4 & 3 \end{pmatrix}$

Now, using corollary 2.1 for computing this block diagonal matrix as following:

From example 4.1 we have: $f(A_1) == \begin{pmatrix} 1.272019649` & -0.7861513777` \\ 0.786151377` & 1.2720196495` \end{pmatrix}$

Follow the same steps as inexample 4.2 we have:

$$f(A_2) = \begin{pmatrix} 1.07675 & -0.451189 & 1.30998 & -0.787252 \\ 1.46716 & 0.760639 & -0.0368473 & 1.72203 \\ 0.142679 & -0.522528 & 1.96089 & -0.831039 \\ -0.400979 & 0.61796 & 1.26498 & 1.63445 \end{pmatrix}$$

Follow the same steps as in example 4.3 we have:

$$f(A_3) = \{\{1.53557, -0.889822 + 5.55112 \times 10^{-17}i, 0.267787, -0.0603337 - 8.88178 \times 10^{-16}i, 2.89255\},$$
$$\{1.51186, 1.13389 - 1.11022 \times 10^{-16}i, 0.755929, 2.12949 - 8.88178 \times 10^{-16}i, 0.808917 - 4.44089 \times 10^{-16}i\},$$
$$\{-0.0474316, 1.40168, 0.976284, 0.805245, 1.61564\}, \{0, 0, 0, 2 + 2.22045 \times 10^{-16}i, -1\}, \{0, 0, 0, 1, 2.22045 \times 10^{-16}i\}\}$$

Now, applying corollary 2.1 we have:

$f(A)$
$= \{\{1.272019649`, -0.7861513777`, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\}, \{0.7861513777`, 1.272019649`, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0\},$

$\{0, 0, 1.07675, -0.451189, 1.30998, -0.787252, 0, 0, 0, 0, 0\}, \{0, 0, 1.46716, 0.760639, -0.0368473, 1.72203, 0, 0, 0, 0, 0\},$

$\{0, 0, 0.142679, -0.522528, 1.96089, -0.831039, 0, 0, 0, 0, 0\}, \{0, 0, -0.400979, 0.61796, 1.26498, 1.63445, 0, 0, 0, 0, 0\},$

$\{1.535, -0.8898 + 5.551 \times 10^{-17} i, 0.2677, -0.06033 - 8.88178 \times 10^{-16} i, 2.892\},$

$\{1.511, 1.133 - 1.11 \times 10^{-16} i, 0.755, 2.12 - 8.88 \times 10^{-16} i, 0.80 - 4.44 \times 10^{-16} i\},$

$\{-0.0474316, 1.40168, 0.976284, 0.805245, 1.61564\}, \{0, 0, 0, 2 + 2.22045 \times 10^{-16} i, -1\}, \{0, 0, 0, 1, 2.22045 \times 10^{-16} i\}\}$

Note: the accuracy of this example is tested as in the previous examples and this example illustrates the matrix functions of square matrices having mixed eigenvalues can be computed using our proposed techniques and methods in this paper.

General remark:In general the proposed methods and technique which we investigated it can be used practically for computing matrix functions of square matrices having complex eigenvalues (pure or mixed) eigenvalues for scalar function defined on the spectrum of a square matrix $A\ (\sigma(A))$as $\cos(A)$, $\sin(A)$, $\cosh(A)$, $\sinh(A)$, e^A, $\ln(A)$, $\sqrt{(A)}$, $(f(A))^{1/n}$and other functions. But in this paper we concentrate on two types of scalar functions square root and exponential function for two reasons, the first of them square root enabled us from test the accuracy of the results of our techniques and the other reason the exponential function used practically in many applications in many applied fields.

5. Conclusion

Computing matrix functions $f(A)$of n-by-n matrix A is a frequently occurring problem in control theory and other applications. In this chapter, we investigated and introduced some formulas for approximating matrix functions for square matrices having (mixed and pure complex) eigenvalues. These new formulas introduced using Newton's divided difference and the interpolation technique. The proposed formulas are tested on several problems especially for square root of square matrices. The obtained results showed that the new approaches are practically and illustrated the applicability of it and showed that it give high accuracy for approximating matrix functions $f(A)$ for square matrices having (mixed or pure complex) eigenvalues. The proposed formulas can be used for solving some important problems in control theory.

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