

Determination of a Matrix Function in the Form of $f(A)=g(q(A))$ Where $g(x)$ Is a Transcendental Function and $q(x)$ Is a Polynomial Function of Large Degree Using the Minimal Polynomial

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Abstract. Matrix functions are used in many areas of linear algebra and arise in numerical applications in science and engineering. In this paper, we introduce an effective approach for determining matrix function $f(A)=g(q(A))$ of a square matrix A , where q is a polynomial function from a degree of m and also function g can be a transcendental function. Computing a matrix function $f(A)$ will be time-consuming and difficult if m is large. We propose a new technique which is based on the minimal polynomial and characteristic polynomial of the given matrix A , which causes, to reduce the degree of polynomial function significantly. The new approach has been tested on several problems to show the efficiency of the presented method. Finally, the application of this method in state space and matrix quantum mechanics is highlighted.

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1. **Introduction**
2. **Preliminary**
3. **Computation of a lower degree polynomial**
4. **Numerical examples**
5. **Application in state space and space of matrix quantum mechanics**
6. **Conclusions**

1. Introduction

Matrix functions are used in many areas of linear algebra and arise in numerical applications in science and engineering such as quantum mechanics, numerical solution of partial differential equations and modern control theory [6,7,8]. Suppose that A is a $n \times n$ matrix and f is an analytical function on spectrum includes A . In numerical articles and books, different methods has been proposed to compute a matrix function [9,10,13,14]. As a result there have been proposed in the literature since 1880 distinct definitions of a matrix function, by Weyr, Sylvester and Buchheim, Giorgi, Cartan, Fantappie', Cipolla, Schwerdtfeger and Richter [5].

The following definitions are the most generally useful for computing a matrix function.

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In Eigenvalue decomposition definition, for any diagonalizable matrix $A = PDP^{-1}$ [2,12], where the eigenvalues in $D = \text{diag}(\lambda_1 I, \lambda_2 I, \dots, \lambda_n I)$ are grouped by repetition. For a function $f(z)$ that is defined at each $\lambda_i \in \lambda(A)$, we define

$$f(A) = Pf(D)P^{-1} = P \text{diag}(f(\lambda_1), f(\lambda_2), \dots, f(\lambda_n))P^{-1}$$

where $\lambda_A = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$. But $A \in \mathbb{C}^{n \times n}$ has the Jordan canonical form [1,11], if we have

$$Z^{-1}AZ = J_A = \text{diag}(J_1(\lambda_1), J_2(\lambda_2), \dots, J_p(\lambda_p)) = \text{diag}(J_1, J_2, \dots, J_p)$$

where Z is a nonsingular matrix and,

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

and $m_1 + m_2 + \dots + m_p = n$. Thus $f(A) := Zf(J_A)Z^{-1} = Z \text{diag}(f(J_k(\lambda_k)))Z^{-1}$, where

$$f(J_k(\lambda_k)) = f(J_k) = \begin{bmatrix} f(\lambda_k) & f'(\lambda_k) & \dots & \frac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ & f(\lambda_k) & \ddots & \\ & & \ddots & f'(\lambda_k) \\ & & & f(\lambda_k) \end{bmatrix}$$

Finally, let A be an $(n+1)$ -by- $(n+1)$ real matrix, where its eigenvalues are not necessarily distinct, $\lambda_A = \{\lambda_0, \lambda_1, \dots, \lambda_n\}$, where $\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_n$, and $f: \mathbb{C} \rightarrow \mathbb{C}$ be defined on λ_A and $f(z)$ be analytic at $z = \lambda_i$ for $i=0, 1, \dots, n$. Now we define $f(A)$ using Newton divided difference and the interpolation technique of Hermite [3] as follows:

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

in which

$$\begin{cases} k[\lambda_i, \dots, \lambda_{i+k}] = f^{(k)}(\lambda_i), & \text{if } \lambda_i = \lambda_{i+k} \\ k[\lambda_i, \dots, \lambda_{i+k}] = \frac{f[\lambda_{i+1}, \dots, \lambda_{i+k}] - f[\lambda_i, \dots, \lambda_{i+k-1}]}{\lambda_{i+k} - \lambda_i}, & \text{otherwise} \end{cases}$$

2. Preliminary

Suppose that $q(x)$ is a polynomial scalar function from degree of m

$$q(x) = b_m x^m + b_{m-1} x^{m-1} + \dots + b_1 x + b_0$$

and also, the characteristic polynomial of $A_{n \times n}$ is

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

Let q be an arbitrary polynomial, in which $\deg q(x) \geq \deg p(x)$ ($m \geq n$). One can compute $q(A)$ by the following method:

By dividing polynomial $q(x)$ in to characteristic polynomial of the matrix A , we

have:

$$q(x) = p(x)t(x) + r(x)$$

so that $t(x)$ and $r(x)$ are quotient polynomial and remainder polynomial, respectively. Since $p(A) = 0$ then $q(A) = r(A)$. So computing of polynomial matrix of degree m lead to computing polynomial matrix of lower degree.

Now we recall the following fundamental theorem and definitions.

Theorem 2.1. Let A be an matrix. If $f(x) = \det(xI - A)$ be characteristic polynomial of matrix A , then we have $f(A) = 0$.

Definition 2.1. [4] Let A be an $n \times n$ matrix. There are many non-zero polynomial for which we have $f(A) = 0$. Among these polynomials, there is the polynomial with the lowest degree in which the leading coefficient is one, in other words it is singularity. Such polynomial $m(t)$ exists and is unique. This polynomial is called minimal polynomial and $m(A) = 0$.

Theorem 2.2. Matrix A is diagonalizable, if and only if, minimal polynomial $m(x)$ will decompose is absolutely without repetition, thus

$$m(x) = (x - c_1)(x - c_2) \dots (x - c_k)$$

where c_1, c_2, \dots, c_k be distinct eigenvalues of matrix A .

Theorem 2.3. The operator $T : V \rightarrow V$ is a diagonalizable operator, when V be a basic such as $B = \{\alpha_1, \alpha_2, \dots, \alpha_n\}$ in which $\alpha_1, \dots, \alpha_n$ are special vectors and also $T(\alpha_1) = c_1\alpha_1, \dots, T(\alpha_n) = c_n\alpha_n$. So it can be said T is diagonalizable when special vectors T created the space V .

3. Computation of a lower degree polynomial

Now, in this section, we consider the computing of matrix function in the form of $f(x) = g(q(x))$ where $q(x)$ is a polynomial of degree m and $g(x)$ is a transcendental function such as exponential and trigonometric function. So in this functions, polynomial functions is used as argument of exponential or trigonometric function, not as the main function. We define a matrix function $f(A) = g(q(A))$ by using characteristic polynomial, minimal polynomial, eigenvalue decomposition and Jordan canonical form. According to Definition 2.1 we concluded that if matrix A is diagonalizable, minimal polynomial can be used instead of characteristic polynomial. Therefore :

$$q(x) = m(x)t^*(x) + r^*(x) \tag{1}$$

Since $m(A) = 0$ then we have

$$q(A) = r^*(A) \tag{2}$$

This has two advantages:

First, it may be $\deg q(x) < \deg p(x)$ (then polynomial $q(x)$ not divisible by characteristic polynomial), but $\deg q(x) \geq \deg m(x)$. Second, the degree of remainder while $q(x)$ divided by $m(x)$ is lower than while $q(x)$ divided by $p(x)$, thus:

$$\deg r^*(x) \leq \deg r(x) \tag{3}$$

Finally, we concluded that employing $m(x)$ instead of $p(x)$ is efficient if matrix A be diagonalizable and eigenvalues is not distinct. But how to distinguish that matrix A is diagonalizable?

We know if the eigenvalues of matrix A are distinct then matrix A is diagonalizable. Now, let think that the eigenvalues of matrix A are not distinct. Suppose that eigenvalue λ_i has an algebraic multiplicity k_i ($i=1, \dots, n$) and matrix A is diagonalizable. Then

$$p(x) = (x - \lambda_1)^{k_1} \dots (x - \lambda_i)^{k_i} \dots (x - \lambda_n)^{k_n}$$

Because matrix A is diagonalizable, then:

$$m(x) = (x - \lambda_1) \dots (x - \lambda_i) \dots (x - \lambda_n)$$

We know from Theorem 2.1 and Definition 2.1 that $p(A) = 0$ and $m(A) = 0$. Thus

$$m(A) = (A - \lambda_1 I) \dots (A - \lambda_i I) \dots (A - \lambda_n I) = 0$$

Moreover

$$(A - \lambda_i I)^{k_i} = c(A - \lambda_i I)$$

where c is an integer and $i=1, \dots, n$.

Eventually if the eigenvalues are not distinct, but

$$(A - \lambda_1 I) \dots (A - \lambda_i I) \dots (A - \lambda_n I) = 0 \quad (4)$$

Matrix A is diagonalizable. Now, suppose that the matrix A is diagonalizable, then we compute matrix function $f(A)$ as follows:

$$q(x) = m(x)t^*(x) + r^*(x) \Rightarrow q(A) = r^*(A)$$

Therefore:

$$f(A) = g(q(A)) = g(r^*(A)) = k(A) \quad (5)$$

On the other hand, according to the Eigenvalue decomposition definition, matrix D can be used instead of matrix A . Thus

$$f(A) = k(A) = Pk(D)P^{-1} \quad (6)$$

where matrix D is diagonal and matrix P is nonsingular.

But if matrix A nondiagonalizable, we use characteristic polynomial. On the other hand, according to the Jordan canonical form definition, J_A can be used instead of A . So we have:

$$q(x) = p(x)t(x) + r(x) \quad (7)$$

$$q(A) = r(A) \quad (8)$$

$$f(A) = g(q(A)) = g(r(A)) = h(A) \quad (9)$$

$$f(A) = h(A) = Xh(J_A)X^{-1} \quad (10)$$

4. Numerical examples

In this section we present several test problem to support the theoretical results.

Example 4.1. Let

$$A = \begin{bmatrix} 7 & -12 & -10 \\ 0 & 1 & 0 \\ 3 & -6 & -4 \end{bmatrix}$$

and $f(x) = \sin(x^4 + 2x)$. We have $\lambda(A) = \{1, 1, 2\}$. By Newton divided difference and the interpolation technique of Hermite definition, we have:

$$\begin{aligned} f(A) &= \sin(A^4 + 2A) = f(\lambda_0)I + f[\lambda_0, \lambda_1](A - \lambda_0 I) + f[\lambda_0, \lambda_1, \lambda_2](A - \lambda_0 I)(A - \lambda_1 I) \\ &= f(1)I + f'(1)(A - I) + f[1, 1, 2](A - I)^2 \\ &= (\sin 3)I + (6 \cos 3)(A - I) + (\sin 20 - \sin 3 - 6 \cos 3)(A - I) \\ &= \begin{bmatrix} -5 \sin 3 + 6 \sin 20 & 12 \sin 3 - 12 \sin 20 & 10 \sin 3 - 10 \sin 20 \\ 0 & \sin 3 & 0 \\ -3 \sin 3 + 3 \sin 20 & 6 \sin 3 - 6 \sin 20 & 6 \sin 3 - 5 \sin 20 \end{bmatrix} \end{aligned}$$

But, we know that A is diagonalizable matrix, thus we have $P^{-1}AP = D$ where

$$P = \begin{bmatrix} 3 & 2 & 2 \\ -1 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}, \quad P^{-1} = \begin{bmatrix} -1 & 2 & 2 \\ -1 & 3 & 2 \\ 3 & -6 & -5 \end{bmatrix}, \quad D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

Furthermore, $p(x) = (x-1)^2(x-2)$ and $m(x) = (x-1)(x-2)$. By applying relation

(2), we have $r^*(x) = 17x - 14$. Thus $k(x) = g(r^*(x)) = \sin(17x - 14)$. Therefore

$$\begin{aligned} k(A) &= \sin(17A - 14I) = Pk(D)P^{-1} \\ &= P \text{diag}(\sin 3, \sin 3, \sin 20)P^{-1} \\ &= \begin{bmatrix} 3 & 2 & 2 \\ -1 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \begin{bmatrix} \sin 3 & 0 & 0 \\ 0 & \sin 3 & 0 \\ 0 & 0 & \sin 20 \end{bmatrix} \begin{bmatrix} -1 & 2 & 2 \\ -1 & 3 & 2 \\ 3 & -6 & -5 \end{bmatrix} \\ &= \begin{bmatrix} -5 \sin 3 + 6 \sin 20 & 12 \sin 3 - 12 \sin 20 & 10 \sin 3 - 10 \sin 20 \\ 0 & \sin 3 & 0 \\ -3 \sin 3 + 3 \sin 20 & 6 \sin 3 - 6 \sin 20 & 6 \sin 3 - 5 \sin 20 \end{bmatrix} \end{aligned}$$

As it seems that the results obtained using both methods are the same and $f(A) = k(A)$.

Example 4.2. Let

$$A = \begin{bmatrix} 5 & -6 & -6 \\ -1 & 4 & 2 \\ 3 & -6 & -4 \end{bmatrix}$$

and $f(x) = e^{x^6 + 2x^4}$. We have $\lambda(A) = \{1, 2, 2\}$. A is a diagonalizable matrix. Thus by defining

$$P = \begin{bmatrix} 3 & 2 & 2 \\ -1 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}, \quad P^{-1} = \begin{bmatrix} -1 & 2 & 2 \\ -1 & 3 & 2 \\ 3 & -6 & -5 \end{bmatrix}, \quad D = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

we have $P^{-1}AP = D$.

On the other hand, $p(x) = (-x+1)(x-2)^2$ and $m(x) = (-x+1)(x-2)$. By applying relation (2), we have $r^*(x) = 93x - 90$. Thus

$$\begin{aligned}
 k(A) &= e^{93A-90I} = Pk(D)P^{-1} = P \operatorname{diag}(e^3, e^{96}, e^{96})P^{-1} \\
 &= 10^{42} \begin{bmatrix} 1.9694 & -2.9541 & -2.9541 \\ -0.4923 & 1.4770 & 0.9847 \\ 1.4770 & -2.9541 & -2.4617 \end{bmatrix}.
 \end{aligned}$$

If we compute $e^{A^6+2A^4}$ using the interpolation technique of Hermite definition, then

$$f(A) = e^{A^6+2A^4} = 10^{42} \begin{bmatrix} 1.9694 & -2.9541 & -2.9541 \\ -0.4923 & 1.4770 & 0.9847 \\ 1.4770 & -2.9541 & -2.4617 \end{bmatrix}.$$

We can see that the values computed using both methods are the same and $f(A) = k(A)$.

Example 4.3. Let

$$A = \begin{bmatrix} 2.2829 & -1.1085 & 0.5233 & 0.9496 & -0.3566 \\ 1.7810 & -1.9845 & 1.8895 & 2.6143 & -2.3062 \\ 2.5 & -4 & 3.5 & 3.5 & -3 \\ 0.5310 & -9.9845 & 0.6395 & 1.8643 & -0.8062 \\ 0.5640 & -0.0930 & -0.0872 & 0.0640 & 1.3372 \end{bmatrix}$$

and $f(x) = \sin(x^8 + 2x^4 + 6)$. We have $\lambda(A) = \{1, 1, 1, 2, 2\}$. By Newton divided difference and interpolation technique of Hermite definition, we have

$$\begin{aligned}
 f(A) &= \sin(A^8 + 2A^4 + 6I) \\
 &= f(\lambda_0)I + f[\lambda_0, \lambda_1](A - \lambda_0 I) + f[\lambda_0, \lambda_1, \lambda_2](A - \lambda_0 I)(A - \lambda_1 I) \\
 &\quad + f[\lambda_0, \lambda_1, \lambda_2, \lambda_3](A - \lambda_0 I)(A - \lambda_1 I)(A - \lambda_2 I) \\
 &\quad + f[\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4](A - \lambda_0 I)(A - \lambda_1 I)(A - \lambda_2 I)(A - \lambda_3 I) \\
 &= (\sin 9)(I) + (16 \cos 9)(A - I) + (40 \cos 9 - 128 \sin 9)(A - I) \\
 &\quad + (\sin 294 + 127 \sin 9 - 56 \cos 9)(A - I) \\
 &= (\sin 9)(I) + (\sin 294 - \sin 9)(A - I) \\
 &= \begin{bmatrix} -1.2161 & 1.1859 & -0.5598 & -1.0159 & 0.3815 \\ -1.9053 & 3.3492 & -2.0214 & -2.7968 & 2.4672 \\ -2.6742 & 4.2792 & -2.5181 & -3.7443 & 3.2094 \\ -0.5681 & 1.0532 & -0.6842 & -0.7683 & 0.8625 \\ -0.6033 & 0.0995 & 0.0933 & -0.0684 & -0.2043 \end{bmatrix}
 \end{aligned}$$

But we know that A is a diagonalizable matrix. Because $(A - I)(A - 2I) = 0$. Thus we have $P^{-1}AP = D$ and

$$P = \begin{bmatrix} -1 & 2 & 2 & 1 & 4 \\ 0 & 6 & -1 & 3 & 1 \\ 2 & 1 & 5 & 4 & 2 \\ 1 & 3 & -7 & 1 & 0 \\ 2 & -2 & -1 & 0 & 3 \end{bmatrix}, \quad D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}.$$

Furthermore, $p(x) = (x-1)^3(x-2)^2$ and $m(x) = (x-1)(x-2)$. By applying relation (2), we have $r^*(x) = 285x - 276$. Thus $k(x) = g(r^*(x)) = \sin(285x - 276)$. Therefore

$$k(A) = \sin(285A - 276I) = Pk(D)P^{-1} = P \text{diag}(\sin 9, \sin 9, \sin 9, \sin 294, \sin 294)P^{-1}$$

$$= \begin{bmatrix} -1.2161 & 1.1859 & -0.5598 & -1.0159 & 0.3815 \\ -1.9053 & 3.3492 & -2.0214 & -2.7968 & 2.4672 \\ -2.6742 & 4.2792 & -2.5181 & -3.7443 & 3.2094 \\ -0.5681 & 1.0532 & -0.6842 & -0.7683 & 0.8625 \\ -0.6033 & 0.0995 & 0.0933 & -0.0684 & -0.2043 \end{bmatrix}.$$

It can be seen that the results obtained using both methods are the same and $f(A) = k(A)$.

Example 4.4. Let

$$A = \begin{bmatrix} -7 & -4 & -3 \\ 10 & 6 & 4 \\ 6 & 3 & 3 \end{bmatrix}$$

and $f(x) = e^{x^5+x}$. We have $\lambda(A) = \{0, 1, 1\}$. A is not diagonalizable. But there are nonsingular matrix X and Jordan matrix J_A , so that $XJ_A X^{-1} = A$ where

$$X = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 2 & 0 \\ -1 & 0 & 3 \end{bmatrix}, \quad J_A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}.$$

Furthermore $p(x) = x(x-1)^2$. By applying relation (7), we have $r(x) = 4x^2 - 2x$ and $h(x) = g(r(x)) = e^{4x^2-2x}$. Thus

$$h(A) = e^{4A^2-2A} = X h(J_A) X^{-1} = X \text{diag}(h(J_k(\lambda_k))) X^{-1}$$

$$= \begin{bmatrix} 1 & -1 & -1 \\ -1 & 2 & 0 \\ -1 & 0 & 3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & e^2 & 6e^2 \\ 0 & 0 & e^2 \end{bmatrix} \begin{bmatrix} 6 & 3 & 2 \\ 3 & 2 & 1 \\ 2 & 1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 6-17e^2 & 3-9e^2 & 2-8e^2 \\ -6+30e^2 & -3+16e^2 & -2+14e^2 \\ -6+6e^2 & -3+3e^2 & -2+3e^2 \end{bmatrix}$$

If we compute e^{A^5+A} using other methods, then we observe that the results are the same and $f(A) = h(A)$.

5. Application in state space and space of matrix quantum mechanics

One of the most important applications of matrixes is in state space. Operators in space of matrix quantum mechanics is in the form of a matrix where impress on states of space and

change them. These operators express sometimes in to a field of matrix and sometimes in to combination of matrixes with different powers. For instance, for transferred a system of quantum mechanics in location space. Operator expresses in to $\exp\left(\frac{iP_x a}{h}\right)$ where is expansionable in to sum of power matrixes. One of most important translation operators is in limited location space in to $F(I) = \exp\left(\frac{-PI}{h}\right)$ where this relation leading to polynomial matrix function from degree of m where m can be large. So, using the new technique presented in this paper, we can easily solve these problems.

6. Conclusions

In this paper, we employed minimal polynomial and characteristic polynomial for computing matrix function $f(A) = g(q(A))$ when g is a transcendental function and q is a polynomial function. The new method was tasted on several problems. The obtained results show that the new approach is efficient. These methods can be used for solving some important problems in state spaces and matrix quantum mechanics, which causes, to reduce the degree of polynomial function significantly. We used the well-known software MATLAB to do the computation.

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