Do the chain rules for matrix functions hold without commutativity?

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Abstract

This paper shows that the commutativity condition $[A(t), A'(t)] = 0$ is often not necessary to guarantee the chain rules for matrix functions: $\frac{d}{dt}f(A(t)) = A'(t)f'(A(t))$ and $\frac{d}{dt}f(A(t)) = f'(A(t))A'(t)$, where $A(t)$ is a square matrix of differentiable functions and f is an analytic function. A further question on the chain rules is presented and discussed.

Keywords: Matrix function; Chain rule; Commutativity; Fundamental matrix solution

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1 Introduction

The chain rules for matrix functions are powerful tools in matrix analysis [1]. In the case of matrix exponential functions, they can yield the exponential representation for the fundamental matrix solutions of homogeneous linear differential equations, and further, the solution formula of the Cauchy problem for linear differential equations. However, the chain rules for matrix functions do not always hold [2]. It is, therefore, important to exemplify the chain rules for matrix functions.

Following Mathias [1], we let D denote an open subset of $\mathbb{R}$ or $\mathbb{C}$, M_n denote the set of $n \times n$ complex matrices and $M_n(D, m)$ denote the set of $n \times n$ complex matrices which have spectrum contained in D and the largest Jordan block of size at most m.

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Let f be an $(m-1)$-times continuously differentiable function over D. Given $A \in M_n(D, m)$, as usual we define the matrix function $f(A)$ as follows:

$$f(A) = r_{A,f}(A), \tag{1.1}$$

where $r_{A,f}$ is any polynomial which interpolates f and its derivatives at the roots of the minimal polynomial of A. That is, if λ is an eigenvalue of A of index k, then

$$f^{(i)}(\lambda) = r_{A,f}^{(i)}(\lambda), \ 0 \le i \le k-1.$$

It follows that $f(A)$ depends on f only through its first few derivatives on the spectrum of A, and

$$(f(A))^T = f(A^T), \tag{1.2}$$

where T denotes the matrix transpose.

Let $A(t) \in M_n(D, m)$ be differentiable on an open interval $I \subset \mathbb{R}$. If f m-times continuously differentiable over D, we can define $f'(A(t))$ as above. Then, the basic property (1.2) on matrix transposes implies that the chain rule for the matrix function $f(A(t))$ holds:

$$\frac{d}{dt}f(A(t)) = A'(t)f'(A(t)) \tag{1.3}$$

if and only if the chain rule for the matrix function $f(A^T(t))$ holds:

$$\frac{d}{dt}f(A^T(t)) = f'(A^T(t))(A^T)'(t). \tag{1.4}$$

Thus, we only need to consider one of the two chain rules: (1.3) and (1.4). Generally, these chain rules need not hold (see Reference [2] or Section 3 for an example). Moreover, if f is $(2m-1)$-times continuously differentiable over D, then we can compute the derivative of $f(A(t))$ with respect to t as follows:

$$\frac{d}{dt}f(A(t)) = \left[f\begin{pmatrix} A(t) & A'(t) \\ 0 & A(t) \end{pmatrix}\right]_{12},$$

where $[\ ]_{12}$ denotes the (1,2) block of the involved matrix [1].

Now let f be analytic and its Maclaurin series $\sum_{i=0}^{\infty} c_i x^i$ converge over D. Then, $f(A(t))$ can be computed by [3]:

$$f(A(t)) = \sum_{i=0}^{\infty} c_i A^i(t). \tag{1.5}$$

Therefore, if $A(t)$ commutes with $A'(t)$, i.e., the commutativity condition:

$$[A(t), A'(t)] = A(t)A'(t) - A'(t)A(t) = 0 \tag{1.6}$$

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is satisfied, then the chain rule (1.3) must hold. A natural question arises: Is the commutativity condition (1.6) necessary to guarantee the chain rule (1.3) for matrix functions?

There is some insightful work by Horn [3] on the relation between

$$[A, B] = AB - BA = 0 \text{ and } e^{A+B} = e^A e^B,$$

where $A, B \in M_n$, in matrix analysis. It is direct to check that the commutativity $[A, B] = 0$ is a sufficient condition for the identities $e^{A+B} = e^A e^B = e^B e^A$ to hold. But it is not necessary, and there are some nice examples (see Chapter 6 of [3]) which tell us that if $[A, B] \neq 0$, then either of the following two statements can be true: (a) three matrices $e^A e^B$, $e^B e^A$ and e^{A+B} are distinct, and (b) two of three matrices $e^A e^B$, $e^B e^A$ and e^{A+B} are the same.

In this paper, we would like to show that the commutativity condition (1.6) is not necessary to guarantee the chain rule (1.3) for matrix functions, either. We will present a class of examples of matrices which satisfy the chain rule (1.3) for matrix functions, but do not satisfy the commutativity condition (1.6). Their transposes also provide examples for the chain rule (1.4) for matrix functions. A further question on the chain rules, which is related to the representation theorem of the fundamental matrix solutions of linear differential equations, will be presented and discussed in the final section.

2 Exploring the chain rules without commutativity

2.1 Matrix exponential function

Let us first consider the chain rule (1.3) for the exponential matrix function:

$$\frac{d}{dt} \exp A(t) = A'(t) \exp A(t), \tag{2.1}$$

where $A(t) \in M_n(D, m)$ is differentiable on an open interval I. We would here like to construct square matrices $A(t)$ which satisfy the chain rule (2.1) but do not satisfy the commutativity condition (1.6).

2.1.1 Complex examples

Let $p \geq 1$, $q \geq 0$, $r \geq 1$ be integers and $n = p + q + r$. We start to present a class of complex square matrices $A(t)$ which satisfy (2.1) but do not satisfy (1.6). These square matrices are given in block form by

$$A(t) := \begin{bmatrix} C & \Theta & F(t) \\ 0 & \Lambda & \Omega \\ 0 & 0 & 0 \end{bmatrix}_{n \times n}, \tag{2.2}$$

where C is a $p \times p$ constant invertible matrix to be determined later, $F(t)$ is a $p \times r$ non-constant differentiable matrix function on the interval I, and Θ, Λ, Ω are $p \times q$, $q \times q$, $q \times r$ constant complex matrices, respectively (if $q = 0$, the matrices Θ, Λ, Ω do not appear in $A(t)$).

On one hand, obviously we have

$$A'(t) = \begin{bmatrix} 0 & 0 & F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}_{n \times n},$$

and then, it is easy to check that

$$[A(t), A'(t)] = \begin{bmatrix} 0 & 0 & CF'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \neq 0, \tag{2.3}$$

since C is invertible and $F'(t) \neq 0$.

On the other hand, observe that

$$A^i(t) = \begin{bmatrix} C^i & \sum_{j=0}^{i-1} C^j \Theta \Lambda^{i-j-1} & C^{i-1}F(t) + \sum_{j=0}^{i-2} C^j \Theta \Lambda^{i-j-2}\Omega \\ 0 & \Lambda^i & \Lambda^{i-1}\Omega \\ 0 & 0 & 0 \end{bmatrix}.$$

It then follows that

$$\exp A(t) = \sum_{i=0}^{\infty} \frac{1}{i!} A^i(t) = \begin{bmatrix} e^C & \sum_{i=1}^{\infty} \frac{1}{i!} \sum_{j=0}^{i-1} C^j \Theta \Lambda^{i-j-1} & G(t) + \sum_{i=2}^{\infty} \frac{1}{i!} \sum_{j=0}^{i-2} C^j \Theta \Lambda^{i-j-2}\Omega \\ 0 & e^\Lambda & \sum_{i=1}^{\infty} \frac{1}{i!} \Lambda^{i-1}\Omega \\ 0 & 0 & I_r \end{bmatrix},$$

where $G(t) = (e^C - I_p)C^{-1}F(t)$ and I_k is the identity matrix of order k, and further,

$$\frac{d}{dt} \exp A(t) = \begin{bmatrix} 0 & 0 & (e^C - I_p)C^{-1}F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Now a direct computation yields

$$\frac{d}{dt} \exp A(t) - A'(t) \exp A(t) = \begin{bmatrix} 0 & 0 & (e^C - C - I_p)C^{-1}F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2.4}$$

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Finally, our assertion (2.1) will follow if we take an invertible complex matrix C such that

$$e^C - C - I_p = 0. \tag{2.5}$$

Let us sum up these results into a compact statement:

Theorem 2.1 *Let $A(t)$ be the matrix defined in block form by (2.2). Then (a) $A(t)$ doesn't commute with $A'(t)$; (b) $A(t)$ satisfies the chain rule (1.3), if C satisfies the matrix equation (2.5); (c) when $p = r = 1$, the chain rule (1.3) holds if and only if the matrix equation (2.5) holds.*

There are plenty of complex matrix solutions to the equation (2.5). Let us check the case of $p = 1$. To solve the equation (2.5), we consider a new equation

$$we^w = -e^{-1}. \tag{2.6}$$

This equation has only one real solution, $w = -1$, but plenty of complex solutions given by values of different brunches of the *Lambert W function* $W(z)$ at the point $z = -e^{-1}$ (cf. [4] and references there). Then, as is easy to see, $c = -w - 1$ gives a non-zero complex solution to (2.5) with $p = 1$. Here are some numerical values for such solutions given by Maple:

$$
\begin{aligned}
c &= \left\{ -\mathrm{LambertW}(k, -e^{-1}) - 1 \mid k \in \mathbb{Z} \right\} \\
&\approx \begin{cases} 2.0888 - 7.4615i & \text{for} \quad k = 1, \\ 2.6641 - 13.879i & \text{for} \quad k = 2, \\ 3.0263 - 20.224i & \text{for} \quad k = 3. \end{cases}
\end{aligned}
$$

A special complex matrix solution to (2.5) is given by

$$C = Q^{-1}\mathrm{diag}(c_1, c_2, \cdots, c_p)Q, \ c_i = -\mathrm{LambertW}(k_i, -e^{-1}) - 1, \ 1 \le i \le p,$$

where $k_1, k_2, \cdots, k_p \ge 0$ are arbitrary integers and Q is an arbitrary invertible complex matrix.

The particular case of $q = 0$ leads to simple block matrices:

$$A(t) = \begin{bmatrix} C & F(t) \\ 0 & 0 \end{bmatrix} \tag{2.7}$$

where C is an invertible complex matrix satisfying (2.5) and $F(t)$ is an arbitrary non-constant differentiable matrix function. In this case, we have

$$\exp A(t) = \begin{bmatrix} e^C & (e^C - I_p)C^{-1}F(t) \\ 0 & I_r \end{bmatrix}$$

and thus, we have

$$\frac{d}{dt}\exp A(t) - A'(t)\exp A(t) = \begin{bmatrix} 0 & (e^C - C - I_p)C^{-1}F'(t) \\ 0 & 0 \end{bmatrix} = 0,$$

but

$$[A(t), A'(t)] = \begin{bmatrix} 0 & CF'(t) \\ 0 & 0 \end{bmatrix} \neq 0.$$

2.1.2   Real examples

Let us now assume that

$$C = (c_{ij})_{p\times p}, \ c_{ij} = a_{ij} + b_{ij}\sqrt{-1}, \ F(t) = (f_{ij}(t))_{p\times r}, \ f_{ij}(t) = g_{ij}(t) + h_{ij}(t)\sqrt{-1}, \quad (2.8)$$

where C is any one of the invertible matrices satisfying (2.5) and $F(t)$ is a non-constant differentiable matrix function. We define two real matrices in two-by-two block form:

$$\bar{C} = (\bar{c}_{ij})_{p\times p}, \ \bar{c}_{ij} = \begin{bmatrix} a_{ij} & b_{ij} \\ -b_{ij} & a_{ij} \end{bmatrix}, \ \bar{F}(t) = (\bar{f}_{ij}(t))_{p\times r}, \ \bar{f}_{ij}(t) = \begin{bmatrix} g_{ij}(t) & h_{ij}(t) \\ -h_{ij}(t) & g_{ij}(t) \end{bmatrix}, \quad (2.9)$$

and introduce a new class of real square matrices

$$A(t) := \begin{bmatrix} \bar{C} & \tilde{\Theta} & \bar{F}(t) \\ 0 & \tilde{\Lambda} & \tilde{\Omega} \\ 0 & 0 & 0 \end{bmatrix}_{n'\times n'}, \quad (2.10)$$

where $\tilde{\Theta}$, $\tilde{\Lambda}$, $\tilde{\Omega}$ are $2p \times s$, $s \times s$, $s \times 2r$ arbitrary constant real matrices, respectively.

A similar computation as above guarantees the chain rule (2.1) for $A(t)$ defined by (2.10) as long as the matrix equation

$$e^{\bar{C}} - \bar{C} - I_{2p} = 0 \quad (2.11)$$

holds. Since $\bar{C}$ and $\bar{F}(t)$ are real matrix representations of the complex matrices C and $F(t)$, $\bar{C}$ is invertible, $e^{\bar{C}}$ is a matrix representation of e^C and $\bar{F}(t)$ is a non-constant differentiable matrix function. It further follows that

$$[A(t), A'(t)] = \begin{bmatrix} 0 & 0 & \bar{C}\bar{F}(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \neq 0, \quad (2.12)$$

and

$$e^{\bar{C}} - \bar{C} - I_{2p} = (d_{ij})_{p\times p}, \ d_{ij} = \begin{bmatrix} \mathrm{Re}(e^{c_{ij}}) - \mathrm{Re}(c_{ij}) - \delta_{ij} & \mathrm{Im}(e^{c_{ij}}) - \mathrm{Im}(c_{ij}) \\ -\mathrm{Im}(e^{c_{ij}}) + \mathrm{Im}(c_{ij}) & \mathrm{Re}(e^{c_{ij}}) - \mathrm{Re}(c_{ij}) - \delta_{ij} \end{bmatrix}, \quad (2.13)$$

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since

$$e^{\bar{C}} = (e^{\bar{c}_{ij}})_{p \times p}, \quad e^{\bar{c}_{ij}} = \begin{bmatrix} \mathrm{Re}(e^{c_{ij}}) & \mathrm{Im}(e^{c_{ij}}) \\ -\mathrm{Im}(e^{c_{ij}}) & \mathrm{Re}(e^{c_{ij}}) \end{bmatrix}.$$

Hence, the equation (2.11) follows from (2.5) through (2.13). This implies that (2.10) defines a class of real square matrices which satisfy the chain rule (2.1) but do not satisfy the commutativity condition (1.6).

Remark 2.1 *The examples above show that the chain rule (2.1) for matrix functions may hold for matrices with a non-commuting relation between $A(t)$ and $A'(t)$. It is interesting to observe that the following equation:*

$$\frac{d}{dt} \exp A(t) = A'(t) \exp A(t) = (\exp A(t)) A'(t) \tag{2.14}$$

implies the commutativity of $A(t)$ and $A'(t)$. Actually, since $A(t)$ commutes with $\exp A(t)$, using $(UV)' = U'V + UV'$, we can differentiate the equation $A(t) \exp A(t) = (\exp A(t)) A(t)$ with respect to t to obtain

$$[A'(t)A(t) - A(t)A'(t)] \exp A(t) = 0.$$

The result follows, since $\exp A(t)$ is invertible for any $A(t)$.

2.2 Matrix power series functions

The method used for the exponential function can be extended to power series functions

$$f(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_n x^n + \cdots, \tag{2.15}$$

which is supposed to converge over D. Then by (1.5), for $A(t)$ defined by (2.2), we have

$$f(A(t)) = \begin{bmatrix} f(C) & \sum\limits_{i=1}^{\infty} c_i \sum\limits_{j=0}^{i-1} C^j \Theta \Lambda^{i-j-1} & G_f(t) + \sum\limits_{i=2}^{\infty} c_i \sum\limits_{j=0}^{i-2} C^j \Theta \Lambda^{i-j-2} \Omega \\ 0 & f(\Lambda) & \sum\limits_{i=1}^{\infty} c_i \Lambda^{i-1} \Omega \\ 0 & 0 & f(0) I_r \end{bmatrix},$$

where $G_f(t) = (f(C) - f(0)I_p)C^{-1}F(t)$. From this, it follows that

$$\frac{d}{dt} f(A(t)) = \begin{bmatrix} 0 & 0 & (f(C) - f(0)I_p)C^{-1}F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

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Now, we have

$$f'(x) = c_1 + 2c_2 x + \cdots + nc_n x^{n-1} + \cdots, \tag{2.16}$$

which converge over D, and thus by (1.5), we arrive at

$$f'(A(t)) = \begin{bmatrix} f(C) & \sum\limits_{i=1}^{\infty} d_i \sum\limits_{j=0}^{i-1} C^j \Theta \Lambda^{i-j-1} & H_f(t) + \sum\limits_{i=2}^{\infty} d_i \sum\limits_{j=0}^{i-2} C^j \Theta \Lambda^{i-j-2} \Omega \\[2ex] 0 & f'(\Lambda) & \sum\limits_{i=1}^{\infty} d_i \Lambda^{i-1} \Omega \\[2ex] 0 & 0 & f'(0) I_r \end{bmatrix},$$

where $d_i = (i+1)c_{i+1}, \ i \geq 1$, and $H_f(t) = (f'(C) - f'(0)I_p)C^{-1}F(t)$. Furthermore, we can compute that

$$\frac{d}{dt} f(A(t)) - A'(t)f'(A(t))$$

$$= \begin{bmatrix} 0 & 0 & (f(C) - f(0)I_p)C^{-1}F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & f'(0)F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & (f(C) - f'(0)C - f(0)I_p)C^{-1}F'(t) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2.17}$$

Summarizing, we obtain the following result on the chain rule (1.3) for matrix power series functions:

Theorem 2.2 *Let $f(x)$ be an analytic function defined by (2.15), and $A(t)$ be the matrix defined in block form by (2.2). Then (a) $A(t)$ doesn't commute with $A'(t)$; (b) $A(t)$ satisfies the chain rule (1.3), if C solves the matrix equation*

$$f(C) - f'(0)C - f(0)I_p = 0; \tag{2.18}$$

(c) when $p = r = 1$, the chain rule (1.3) holds if and only if the equation (2.18) holds.

When a matrix solution C of (2.18) is complex, use real matrix representations of C and $F(t)$ to obtain a real matrix $A(t)$ of the form (2.10) that satisfies (1.3) and $[A(t), A'(t)] \neq 0$.

Let $p = 1$. As an example of (2.10), we can easily see that the matrix of the form (2.10) with $C \neq 0$ exists for $f(x) = c_0 + c_1 x + c_2 x^2$ if and only if $c_2 = 0$. Moreover, if $\phi(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$ and $c_2 \neq 0$ and $c_3 \neq 0$, then the matrix of the form (2.10) with $C = -\frac{c_2}{c_3}$ satisfies (1.3) and $[A(t), A'(t)] \neq 0$.

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Remark 2.2 *It is also interesting to examine those classes of sufficiently differentiable (cf. [1]) functions f for which (1.3) implies the commutativity of $A(t)$ and $A'(t)$, i.e., (1.6). First, it is clearly not so for linear functions f, since for these functions, (1.3) holds for all $A(t)$. Second, it is easy to see that for $f(x) = x^2$, the chain rule*

$$\frac{d}{dt}A^2(t) = 2A'(t)A(t)$$

implies the commutativity condition (1.6), since we have $\frac{d}{dt}A^2(t) = A'(t)A(t) + A(t)A'(t)$.

3   A further question

Let us finally observe a system of linear differential equations on an interval $I = (a, b) \subseteq \mathbb{R}$:

$$\dot{x}(t) = A(t)x(t) + f(t), \tag{3.1}$$

where $f(t) \in \mathbb{R}^n$ is continuous on I and $A(t)$ is an $n \times n$ matrix of real continuous functions on I. An important question in differential equations is how to solve (or present the solution to) the Cauchy problem of the system:

$$\dot{x}(t) = A(t)x(t) + f(t), \ x(t_0) = x_0, \tag{3.2}$$

where $t_0 \in I$ and $x_0 \in \mathbb{R}^n$ are given. Examples of solving differential equations, including linear differential equations with constant coefficients, can be founded, for example, in [5, 6].

Generally, it is direct to show that if the matrix $A(t)$ commutes with its integral $\int_{t_0}^t A(s)\,ds$:

$$[A(t), \int_{t_0}^t A(s)\,ds] = 0, \ t \in I, \tag{3.3}$$

then the fundamental matrix solution $U(t, t_0)$ of the homogeneous system $\dot{x}(t) = A(t)x(t)$ is determined by

$$U(t, t_0) = \exp \int_{t_0}^t A(s)\,ds, \ t \in I. \tag{3.4}$$

This means that if we have the commutativity condition (3.3), the following chain rule holds:

$$\frac{d}{dt} \exp \int_{t_0}^t A(s)\,ds = A(t) \exp \int_{t_0}^t A(s)\,ds, \ t \in I. \tag{3.5}$$

This further implies that the unique solution to the Cauchy problem (3.2) is given by the variation of parameters formula:

$$x(t) = U(t, t_0)x_0 + \int_{t_0}^t U(t, s)f(s)\,ds, \ t \in I. \tag{3.6}$$

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However, if we do not have the commutativity condition (3.3), then we cannot expect to have the aforementioned chain rule (3.5). A simple example is given by

$$A(t) = \begin{bmatrix} t & 1 \\ 0 & 0 \end{bmatrix}. \tag{3.7}$$

It is direct to see that

$$\exp \int_0^t A(s)\,ds = \begin{bmatrix} e^{t^2/2} & \frac{2}{t}(e^{t^2/2} - 1) \\ 0 & 1 \end{bmatrix}, \tag{3.8}$$

and so, the chain rule (3.5) does not hold for the matrix $A(t)$ defined by (3.7) (see [2] for more details).

Now, it is natural to ask if the commutativity condition (3.3) is necessary to guarantee the chain rule (3.5). Namely, is there any matrix $A(t)$ of real continuous functions, which satisfies (3.5) but does not satisfy (3.3)? This is more general than the question we discussed in the preceding section, since $\frac{d}{dt} \int_{t_0}^t A(s)\,ds = A(t)$. Any answer will provide an important supplement to the representation theorem of fundamental matrix solutions of linear differential equations with variable-coefficients.

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