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On the Inverse of the Caputo Matrix Exponential

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Abstract: Matrix exponentials are widely used to efficiently tackle systems of linear differential equations. To be able to solve systems of fractional differential equations, the Caputo matrix exponential of the index $\alpha > 0$ was introduced. It generalizes and adapts the conventional matrix exponential to systems of fractional differential equations with constant coefficients. This paper analyzes the most significant properties of the Caputo matrix exponential, in particular those related to its inverse. Several numerical test examples are discussed throughout this exposition in order to outline our approach. Moreover, we demonstrate that the inverse of a Caputo matrix exponential in general is not another Caputo matrix exponential.

Keywords: Caputo matrix exponential; matrix inverse; fractional derivative

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1. Introduction and Motivation

Formally a square matrix $A \in \mathbb{C}^{r \times r}$ can be associated with its exponential matrix function e^{At}. The traditional matrix exponential takes a prominent position among all matrix functions—ultimately due to its relevance in the resolution of systems of first-order ordinary differential equations. However, in practice its efficient numerical computation poses considerable difficulties, see [1] for details.

At the same time, systems of fractional differential equations, which contain derivatives extending the standard integer-order derivative to arbitrary order $\alpha \geq 0$, play an important role in many other important applications of science and engineering [2–4]. Although fractional calculus is factually known since the end of the 17th century [5], only during the recent decades its relevance for practical modeling and engineering simulations has become evident. Fractional derivatives naturally implement Volterra's "principle of the dissipation of hereditary action", meaning that causality aspects and memory characteristics of dynamical systems may easily be incorporated. Important applications are in hydrology, e.g., flow simulations of fluids in porous media, and in civil engineering, e.g., traffic flow problems on road networks, among many others [6,7].

A great variety of fractional derivatives are proposed and used in the literature. The most common fractional derivative is the derivative introduced by Caputo [8]. It is defined in terms of the Riemann–Liouville fractional integral of order $\alpha \geq 0$ operating on function $f(t)$:

$$J^{\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau)\, d\tau, \quad t > 0.$$

Then, provided that f is a locally integrable function, the following operation on f defines its fractional derivative of Caputo with order $\alpha \geq 0$:

$$D^{\alpha} f(t) = J^{m-\alpha} D^{m} f(t), \quad t > 0, \quad m-1 < \alpha \leq m, \quad m \in \mathbb{N}.$$

Note that, as expected, $D^n = d^n/dt^n$ agrees with the usual derivative of integer order $n \in \mathbb{N}$. (Our convention is to use $\mathbb{N}$ for the set of all positive integer numbers, whereas $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.)

In 2016, Rodrigo [9] introduced the fractional exponential matrix of Caputo of order $\alpha \geq 0$. Similarly, here we are using the following definition for $0 \leq \alpha \leq 1$:

$$\exp_{\star}\left(t^{\alpha} A; \alpha\right) = \sum_{n \geq 0} \frac{A^n t^{\alpha n}}{\Gamma(\alpha n + 1)}, \quad t > 0, \tag{1}$$

in relation with the Mittag–Leffler matrix function [10].

It is well-known that inverse problems [11] are among the most basic applications for the inverse of the conventional exponential matrix. Moreover, mathematical optimisation is another area in which the inverse of the matrix exponential is frequently encountered and of significant relevance, see, e.g., (Reference [12], Equations (4.4) and (4.7)). Observe that if in a linear differential system all ordinary derivatives are replaced by fractional derivatives of Caputo type, then the associated inverse problems will necessarily involve the inverse of the Caputo matrix exponential.

In the case of the Caputo matrix exponential, (1), there still remains to clarify the existence of its inverse, in full analogy to the case of the conventional matrix exponential e^{At} with inverse matrix e^{-At}. The final objective of this work will be to study the existence and computation of the inverse of the Caputo matrix exponential.

The present paper is organized as follows. Section 2 first focuses on checking the main properties of the matrix exponential of Caputo, and also on presenting counterexamples of other questionable properties which eventually are not satisfied. In Section 3, we will demonstrate that, in general, the inverse of an exponential matrix of Caputo is not another exponential matrix of Caputo. Finally, Section 4 concludes with the actual computation of the inverse of the Caputo matrix exponential and gives examples.

In the remainder of this work, we will denote by $\mathbb{C}^{p \times q}$ the set of rectangular complex matrices. For a square matrix $A \in \mathbb{C}^{r \times r}$, as usual $\sigma(A)$ denotes the spectrum of matrix A, i.e., the set of its eigenvalues. Moreover, we will denote by $\|A\|$ any multiplicative norm of matrix A. In particular, $\|A\|_2$ is the 2-norm, defined by

$$\|A\|_2 = \sup_{z \neq 0} \frac{\|Az\|_2}{\|z\|_2},$$

where for any vector $z \in \mathbb{C}^q$, the usual Euclidean norm of z is $\|z\|_2 = (z^t z)^{1/2}$. Additionally, it will be helpful to remember that for a family of matrices $\mathcal{A}(k,n) \in \mathbb{C}^{r \times r}$ with n and k being positive, the following identity holds

$$\sum_{n \geq 0} \sum_{k \geq 0} \mathcal{A}(k,n) = \sum_{n \geq 0} \sum_{k=0}^{n} \mathcal{A}(k, n-k). \tag{2}$$

This identity is analogous to the one of the proof for Lemma 11 in (Reference [13], p. 57).

2. Caputo Matrix Exponential

This section first presents some of the fundamental properties of the Caputo matrix exponential which will be built upon in subsequent parts of this work. Then, the next subsection concentrates on some striking counterexamples of properties which one could naively intuit but which at the end do not hold. The final subsection centers on the existence of the inverse of the Caputo matrix exponential and its conditions.

2.1. Properties

In the following, we list the most important fundamental properties of the Caputo matrix exponential which unreservedly have to be fulfilled:

(a) For $\alpha = 1$, the Caputo matrix exponential coincides with the conventional matrix exponential:

$$\exp_\star(tA;1) = e^{At}. \tag{3}$$

(b) If $0_{r\times r}, I_{r\times r}$ are the null and identity matrices of $\mathbb{C}^{r\times r}$, respectively, it is clear that

$$\exp_\star(0_{r\times r};\alpha) = I_{r\times r}. \tag{4}$$

(c) If $A \in \mathbb{C}^{r\times r}$, and $\sigma(A)$ denotes the set of its eigenvalues, it is well known that A has the Jordan canonical factorization $A = PJP^{-1}$, where J is a diagonal block-matrix given by

$$J = \operatorname{diag}\{J_1, J_2, \ldots, J_k\}, \quad J_i = \begin{pmatrix} \lambda_i & 1 & & \mathbf{0} \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ \mathbf{0} & & & \lambda_i \end{pmatrix}, \quad \lambda_i \in \sigma(A).$$

Then from Definition (1), it immediately follows that

$$\exp_\star(t^\alpha A;\alpha) = P \operatorname{diag}\left\{ \exp_\star(t^\alpha J_1;\alpha), \exp_\star(t^\alpha J_2;\alpha), \ldots, \exp_\star(t^\alpha J_k;\alpha) \right\} P^{-1}. \tag{5}$$

(d) Avoiding entirely the Jordan canonical form of A and only knowing $\sigma(A)$, Putzer's method (see e.g., [9]) allows to explicitly obtain $\exp_\star(t^\alpha A;\alpha)$ in fully analytical form.

2.2. Counterexamples

However, there are obvious differences between $\exp_\star(t^\alpha A;\alpha)$ and the matrix exponential e^{At}, which are straightforward to detect considering the scalar case $r = 1$.

(1) The matrix exponential e^{At} is a periodic function of period $T = 2\pi i\, I_{r\times r}$, where i as usual is the imaginary unit:

$$e^{At} = e^{At+2\pi i I_{r\times r}}.$$

However, this is not the case for the Caputo matrix exponential, even in the scalar case ($r = 1$). In fact, it easily can be checked that for $A = 1, t = 1$ and $\alpha = 1/2$, we have

$$\begin{aligned} \exp_\star(1;1/2) &\approx 5.00898 \\ \exp_\star(1+2\pi i;1/2) &\approx -0.0144688 + 0.0885799i, \end{aligned}$$

so that

$$\exp_\star(1;1/2) \neq \exp_\star(1+2\pi i;1/2).$$

Thus, we generally conclude that

$$\exp_\star(A;\alpha) \neq \exp_\star(A + 2\pi i I_{r\times r};\alpha). \tag{6}$$

(2) It is well known that if A and B are two commuting matrices, i.e., $AB = BA$, then

$$e^{(A+B)t} = e^{At}e^{Bt}. \tag{7}$$

This relation is generally not true for the fractional exponential matrix of Caputo—even for the simplest scalar case ($r = 1$). In fact, we can easily observe that when we take $A = B = 1$, $t = 1, \alpha = 1/2$, we have

$$\begin{aligned} \exp_\star(1; 1/2) &\approx 5.00898 \\ \exp_\star(2; 1/2) &\approx 108.941, \end{aligned}$$

so that

$$\exp_\star(2; 1/2) \neq \exp_\star(1; 1/2)\exp_\star(1; 1/2).$$

Consequently, we generally have

$$\exp_\star(t^\alpha(A+B); \alpha) \neq \exp_\star(t^\alpha A; \alpha)\exp_\star(t^\alpha B; \alpha), \tag{8}$$

and the Caputo matrix exponential therefore does not satisfy the semigroup property.

(3) If we denote by $\mathrm{Det}(A)$ the determinant of the square matrix A and by $\mathrm{Tr}(A)$ its trace, i.e., the sum of the elements on the main diagonal, it is well known that the matrix exponential satisfies

$$\mathrm{Det}\left(e^A\right) = e^{\mathrm{Tr}(A)}. \tag{9}$$

In this way, it becomes obvious that the usual exponential matrix e^A is always invertible, since its determinant is always non-zero. Observe that the analogous identity for the Caputo matrix exponential is not true, i.e., $\mathrm{Det}(\exp_\star(A; \alpha)) \neq \exp_\star(\mathrm{Tr}(A); \alpha)$. To prove that this property is not true, it is easy to check that

$$\exp_\star\left(t^\alpha \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; \alpha\right) = \begin{pmatrix} \frac{4}{3}E_\alpha(t^\alpha) - \frac{1}{3}E_\alpha(-2t^\alpha) & \frac{1}{3}E_\alpha(-2t^\alpha) - \frac{1}{3}E_\alpha(t^\alpha) \\ \frac{4}{3}E_\alpha(t^\alpha) - \frac{4}{3}E_\alpha(-2t^\alpha) & \frac{4}{3}E_\alpha(-2t^\alpha) - \frac{1}{3}E_\alpha(t^\alpha) \end{pmatrix},$$

where $E_\alpha(z)$ is the Mittag-Leffler function defined by

$$E_\alpha(z) = \sum_{j \geq 0} \frac{z^j}{\Gamma(\alpha j + 1)}. \tag{10}$$

Now, taking $t = 1, \alpha = 1/2$ and $\mathrm{Tr}\begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix} = -1$, one gets that

$$\mathrm{Det}\left(\exp_\star\left(\begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; 1/2\right)\right) \approx 1.27927, \; \exp_\star(-1; 1/2) \approx 0.427584,$$

so that in general

$$\mathrm{Det}(\exp_\star(A; \alpha)) \neq \exp_\star(\mathrm{Tr}(A); \alpha).$$

(4) As a consequence of (7), it follows that for $A \in \mathbb{C}^{r \times r}$ it is

$$e^{At}e^{-At} = I_{r \times r}. \tag{11}$$

For this reason the exponential matrix e^{At} is always invertible, and its inverse is precisely e^{-At}. On the other hand, for the inverse of the Caputo matrix exponential, it is easy to verify that property (11) is not fulfilled.

As an example, we consider the two matrix exponentials

$$\exp_\star\left(t^\alpha \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; \alpha\right) = \begin{pmatrix} \frac{4}{3}E_\alpha(t^\alpha) - \frac{1}{3}E_\alpha(-2t^\alpha) & \frac{1}{3}E_\alpha(-2t^\alpha) - \frac{1}{3}E_\alpha(t^\alpha) \\ \frac{4}{3}E_\alpha(t^\alpha) - \frac{4}{3}E_\alpha(-2t^\alpha) & \frac{4}{3}E_\alpha(-2t^\alpha) - \frac{1}{3}E_\alpha(t^\alpha) \end{pmatrix}$$

and

$$\exp_\star\left(-t^\alpha\begin{pmatrix}2 & -1\\ 4 & -3\end{pmatrix};\alpha\right)=\begin{pmatrix}\frac{4}{3}E_\alpha\left(-t^\alpha\right)-\frac{1}{3}E_\alpha\left(2t^\alpha\right) & \frac{1}{3}E_\alpha\left(2t^\alpha\right)-\frac{1}{3}E_\alpha\left(-t^\alpha\right)\\ \frac{4}{3}E_\alpha\left(-t^\alpha\right)-\frac{4}{3}E_\alpha\left(2t^\alpha\right) & \frac{4}{3}E_\alpha\left(2t^\alpha\right)-\frac{1}{3}E_\alpha\left(-t^\alpha\right)\end{pmatrix}.$$

For the choice $\alpha = 1/2$ with $t = 1$, we obtain

$$\exp_\star\left(\begin{pmatrix}2 & -1\\ 4 & -3\end{pmatrix};1/2\right)\exp_\star\left(-\begin{pmatrix}2 & -1\\ 4 & -3\end{pmatrix};1/2\right)\approx\begin{pmatrix}-6.41867 & 8.56043\\ -34.2417 & 36.3835\end{pmatrix}\neq I_{2\times 2},$$

and it clearly is

$$\exp_\star\left(t^\alpha A;\alpha\right)\exp_\star\left(-t^\alpha A;\alpha\right)\neq I_{r\times r}.$$

2.3. Existence

In order to guarantee the existence of the inverse of the Caputo matrix exponential $\exp_\star\left(t^\alpha A;\alpha\right)$ for $A\in\mathbb{C}^{r\times r}$, observe that from definition (1), for $\alpha>0, t\geq 0$, it follows that

$$\left\|I_{r\times r}-\exp_\star\left(t^\alpha A;\alpha\right)\right\|=\left\|\sum_{n\geq 1}\frac{A^n t^{\alpha n}}{\Gamma\left(\alpha n+1\right)}\right\|\leq\sum_{n\geq 1}\frac{\left(\|A\|\,t^\alpha\right)^n}{\Gamma\left(\alpha n+1\right)}=E_\alpha\left(\|A\|\,t^\alpha\right)-1.$$

Then, according to Lemma 2.3.3 in (Ref. [14], p. 58), matrix $\exp_\star\left(t^\alpha A;\alpha\right)$ is invertible in the interval $I=[0,t^\star]$, where

$$E_\alpha\left(\|A\|\,t^\alpha\right)<2. \tag{12}$$

Taking into account that the Mittag–Leffler function $g(t)=E_\alpha\left(\|A\|\,t^\alpha\right)$ satisfies $g(0)=1$, and it is a strictly increasing function for $t\in(0,+\infty)$, we can conclude that there always exists $t^\star$ so that inequality (12) holds in $I=[0,t^\star]$. Therefore, $\exp_\star\left(t^\alpha A;\alpha\right)^{-1}$ also exists, at least for $t\in I$.

Example 1. *For the particular case* $A=\begin{pmatrix}2 & -1\\ 4 & -3\end{pmatrix}$ *and also index* $\alpha=1/4$, *it is easy to check that* $\|A\|_2\approx 5.46499$. *Then, it holds*

$$E_{0.25}\left(5.46499\,t^{1/4}\right)<2\;\Leftrightarrow\; t\in[0,0.0000594].$$

Thus, if $t\in[0,0.0000594]$, *the inverse* $\exp_\star\left(t^{1/4}\begin{pmatrix}2 & -1\\ 4 & -3\end{pmatrix};1/4\right)^{-1}$ *exists.*

3. A New Inversion Property of the Caputo Matrix Exponential

In Section 2.3, we proved the existence of the inverse of the Caputo matrix exponential. It is well-known that the inverse of the conventional matrix exponential e^{At} is again an exponential of the matrix $-At$, or simply $\left(e^{At}\right)^{-1}=e^{-At}$. So can we arrive at a similar property for the Caputo matrix exponential?

For this purpose, let us consider the matrix

$$A=\begin{pmatrix}0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\end{pmatrix}. \tag{13}$$

The square matrix A is a nilpotent matrix of index 3, meaning that $A^3 \neq 0_{4\times 4}$ but $A^n = 0_{4\times 4}$ for $n \geq 4$. Thus, applying Definition (1), it is easy to establish

$$\exp_\star(t^\alpha A;\alpha) = \sum_{n=0}^{3} \frac{A^n t^{\alpha n}}{\Gamma(n\alpha+1)} = \begin{pmatrix} 1 & \frac{t^\alpha}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} & \frac{t^{3\alpha}}{\Gamma(3\alpha+1)} \\ 0 & 1 & \frac{t^\alpha}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} \\ 0 & 0 & 1 & \frac{t^\alpha}{\Gamma(\alpha+1)} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Now, we proceed to calculate its inverse and obtain

$$\exp_\star(t^\alpha A;\alpha)^{-1} = \begin{pmatrix} 1 & -\frac{t^\alpha}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(\alpha+1)^2} - \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} & -\frac{t^{3\alpha}}{\Gamma(\alpha+1)^3} + \frac{2t^{3\alpha}}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \frac{t^{3\alpha}}{\Gamma(3\alpha+1)} \\ 0 & 1 & -\frac{t^\alpha}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(\alpha+1)^2} - \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} \\ 0 & 0 & 1 & -\frac{t^\alpha}{\Gamma(\alpha+1)} \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{14}$$

Suppose that there exists a matrix $B \in \mathbb{C}^{4\times 4}$ such that

$$\exp_\star(t^\alpha A;\alpha)^{-1} = \exp_\star(t^\alpha B;\alpha) = \sum_{n\geq 0} \frac{B^n t^{\alpha n}}{\Gamma(n\alpha+1)}. \tag{15}$$

Then, we may recast the expression for the inverse given by (14) in the form

$$\begin{aligned} \exp_\star(t^\alpha A;\alpha)^{-1} = \quad & I_{4\times 4} - \tfrac{1}{\Gamma(\alpha+1)} \begin{pmatrix} 0&1&0&0\\0&0&1&0\\0&0&0&1\\0&0&0&0 \end{pmatrix} t^\alpha + \left(\tfrac{1}{\Gamma(\alpha+1)^2} - \tfrac{1}{\Gamma(2\alpha+1)}\right) \begin{pmatrix} 0&0&1&0\\0&0&0&1\\0&0&0&0\\0&0&0&0 \end{pmatrix} t^{2\alpha} \\ & + \left(-\tfrac{1}{\Gamma(\alpha+1)^3} + \tfrac{2}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \tfrac{1}{\Gamma(3\alpha+1)}\right) \begin{pmatrix} 0&0&0&1\\0&0&0&0\\0&0&0&0\\0&0&0&0 \end{pmatrix} t^{3\alpha} \\ = \quad & I_{4\times 4} - \frac{1}{\Gamma(\alpha+1)} A t^\alpha + \left(\frac{1}{\Gamma(\alpha+1)^2} - \frac{1}{\Gamma(2\alpha+1)}\right) A^2 t^{2\alpha} \\ & + \left(-\frac{1}{\Gamma(\alpha+1)^3} + \frac{2}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \frac{1}{\Gamma(3\alpha+1)}\right) A^3 t^{3\alpha}. \end{aligned} \tag{16}$$

Equating the powers of t^α in (15) and (16), we observe that matrix B must satisfy the following system

$$\left.\begin{aligned} B &= -A \\ B^2 &= \Gamma(2\alpha+1)\left(\frac{1}{\Gamma(\alpha+1)^2} - \frac{1}{\Gamma(2\alpha+1)}\right) A^2 \\ B^3 &= \Gamma(3\alpha+1)\left(-\frac{1}{\Gamma(\alpha+1)^3} + \frac{2}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \frac{1}{\Gamma(3\alpha+1)}\right) A^3 \end{aligned}\right\}. \tag{17}$$

Eliminating recursively all matrices of the previous system yields

$$\left.\begin{aligned} \Gamma(2\alpha+1)\left(\frac{1}{\Gamma(\alpha+1)^2} - \frac{1}{\Gamma(2\alpha+1)}\right) &= 1 \\ \Gamma(3\alpha+1)\left(-\frac{1}{\Gamma(\alpha+1)^3} + \frac{2}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \frac{1}{\Gamma(3\alpha+1)}\right) &= -1 \end{aligned}\right\}. \tag{18}$$

If the first equation of (18) holds, i.e., $\alpha > 0$ satisfies

$$\frac{\Gamma(2\alpha+1)}{\Gamma(\alpha+1)^2} = 2, \tag{19}$$

then the second equation of (18) also holds. Equation (19) has the unique solution $\alpha = 1$, and therefore also system (17). In consequence—except for the trivial case $\alpha = 1$—we affirm that the inverse of the Caputo matrix exponential generally is not another Caputo matrix exponential.

4. On the Computation of the Inverse of the Caputo Matrix Exponential

We now propose to determine the inverse of the Caputo matrix exponential. For this, we introduce the following definition:

Definition 1. *Let $A \in \mathbb{C}^{r\times r}$ be an arbitrary square matrix and $\alpha > 0$. We define the sequence of matrices $\{D_n(\alpha)\}_{n\geq 0}$ as*

$$D_0(\alpha) = I_{r\times r}, \quad D_n(\alpha) = -\sum_{k=0}^{n-1} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]}, \quad n \geq 1. \tag{20}$$

We are now in the position to proceed with the following theorem, which is a refinement of the arguments already presented in Section 2.3, explaining why the inverse of $\exp_\star(t^\alpha A;\alpha)$ exists for $t > 0$, though sufficiently small, and satisfying inequality (12).

Theorem 1. *Let $A \in \mathbb{C}^{r\times r}$ be a square matrix and $0 < \alpha \leq 1$. Let $t > 0$ be such that the fractional matrix function $f(t,\alpha)$, defined by*

$$f(t,\alpha) = \sum_{n\geq 0} D_n(\alpha) t^{n\alpha}, \tag{21}$$

converges. Then, it holds

(a) $\exp_\star(t^\alpha A;\alpha)\, f(t,\alpha) = I_{r\times r}$,

(b) $f(t,\alpha) \exp_\star(t^\alpha A;\alpha) = I_{r\times r}$.

Proof of Theorem 1. For the proof of convergence of $f(t,\alpha)$, recall that asymptotically

$$\Gamma(n\alpha+1) \sim \sqrt{2\pi}\, e^{-\alpha n} (\alpha n)^{\alpha n+\frac{1}{2}}, n \to \infty,$$

so that we conclude

$$\lim_{n\to\infty} \frac{\Gamma(n\alpha+1)^{1/n}}{n^\alpha} = e^{-\alpha}\alpha^\alpha.$$

Hence, the series

$$\sum_{n\geq 1} \frac{z^n A^n}{\Gamma(n\alpha+1)}$$

converges for all $z \in \mathbb{C}$. This convergence occurs uniformly on compact subsets of $\mathbb{C}$. Therefore, the set

$$\left\{ z \in \mathbb{C} : \sup_{\lambda\in\sigma(A)} \left| \sum_{n\geq 1} \frac{z^n \lambda^n}{\Gamma(n\alpha+1)} \right| < 1 \right\}$$

contains a circular disc centered at the origin, $D(0, r(A,\alpha))$, with radius $r(A,\alpha) > 0$. This radius can be determined by considering the Mittag-Leffler function already introduced in (10), specifically $E_\alpha(z\lambda)$ for $z, \lambda \in \mathbb{C}$, which is analytic.

By the spectral mapping theorem, if $A \in \mathbb{C}^{r\times r}$, the spectrum $\sigma(E_\alpha(zA))$ of $E_\alpha(zA) \in \mathbb{C}^{r\times r}$ satisfies

$$\sigma(E_\alpha(zA)) = \{E_\alpha(z\lambda) : \lambda \in \sigma(A)\}.$$

If A is not a nilpotent matrix, then $\sup\{|\lambda| : \lambda \in \sigma(A)\} > 0$. In this case, we choose

$$\begin{aligned} r(A,\alpha) &= \inf\{|z| : E_\alpha(z\lambda) = 0 \text{ for some } \lambda \in \sigma(A)\} \\ &= \inf\left\{\frac{|w|}{|\lambda|} : E_\alpha(w) = 0, w \in \mathbb{C}, \lambda \in \sigma(A)\right\} \\ &= \frac{\inf\{|w| : E_\alpha(w) = 0, w \in \mathbb{C}\}}{\sup\{|\lambda| : \lambda \in \sigma(A)\}} > 0 \end{aligned}$$

because $E_\alpha(0) = 1$. Moreover, the series $\sum_{n\geq 0} D_n(\alpha) z^n$ converges for $|z| < r(A,\alpha)$, because on the disc $D(0, r(A,\alpha))$ the matrix function $E_\alpha(zA)$ is invertible and analytic in $\mathbb{C}$.

If A is a nilpotent matrix, i.e., $\sigma(A) = \{0\}$, and has index $k \in \mathbb{N}$, then $D_n(\alpha)$ defined in (20) vanishes when $n \geq k$. Thus, series (21) only has a finite number of terms and apparently converges.

Now, we proceed with the remainder of the Theorem 1, proving part (a).

(a) Applying the respective Definitions (1) and (21), we compute

$$\begin{aligned} \exp_\star(t^\alpha A;\alpha) f(t,\alpha) &= \left(\sum_{n\geq 0} \frac{A^n t^{n\alpha}}{\Gamma(\alpha n+1)}\right)\left(\sum_{k\geq 0} D_k(\alpha) t^{k\alpha}\right) \\ &= \sum_{n\geq 0}\sum_{k\geq 0} \frac{A^n D_k(\alpha) t^{k\alpha} t^{\alpha n}}{\Gamma(\alpha n+1)}, \text{ taking } \mathcal{A}(n,k) = \frac{A^n D_k(\alpha) t^{k\alpha} t^{\alpha n}}{\Gamma(\alpha n+1)} \text{ of (2)}, \\ &= \sum_{n\geq 0}\sum_{k=0}^{n} \frac{A^{n-k} D_k(\alpha) t^{k\alpha} t^{(n-k)\alpha}}{\Gamma[(n-k)\alpha+1]} = \sum_{n\geq 0}\left(\sum_{k=0}^{n} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]}\right) t^{n\alpha} \\ &= D_0(\alpha) + \sum_{n\geq 1}\left(\sum_{k=0}^{n} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]}\right) t^{n\alpha} \\ &= I_{r\times r} + \sum_{n\geq 1}\left(\sum_{k=0}^{n-1} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]} + D_n(\alpha)\right) t^{n\alpha} \\ &= I_{r\times r} + \sum_{n\geq 1}\left(\sum_{k=0}^{n-1} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]} - \sum_{k=0}^{n-1} \frac{A^{n-k} D_k(\alpha)}{\Gamma[(n-k)\alpha+1]}\right) t^{n\alpha} \\ &= I_{r\times r}. \end{aligned}$$

(b) This equality is equivalent to (a), because the matrix operators $\exp_\star(t^\alpha A;\alpha)$ and $f(t,\alpha)$ commute. In fact, let $f(z)$ and $g(z)$ be holomorphic functions of the complex variable z, both defined on an open set $\Omega \subset \mathbb{C}$. Further, let matrix $A \in \mathbb{C}^{r\times r}$ be such that $\sigma(A) \in \Omega$. Then, from the properties of the matrix functional calculus ([15], p. 558), it follows $f(A)g(A) = g(A)f(A)$.

□

Remark 1. *Following the same line of argument of this proof, a result similar to that of Theorem 1 is also valid for bounded operators A acting in a complex Banach space. One requires the well-known fact that $\sigma(A) \in \mathbb{C}$ is non-void and compact together with the equality*

$$\sup\{|\lambda| : \lambda \in \sigma(A)\} = \limsup_{n\to\infty} \|A^n\|^{1/n}.$$

Then, if A is quasi-nilpotent, it follows $\sup\{|\lambda| : \lambda \in \sigma(A)\} = 0$, and thus $r(A,\alpha) = \infty$.

Remark 2. *Note that the sequence* $\{D_n(\alpha)\}_{n\in\mathbb{N}_0}$ *in Formula* (20) *may be recast into the following compact expression*

$$D_n(\alpha) = A^n \sum_{\ell=1}^{n} (-1)^\ell \sum_{n_1+\ldots+n_\ell=n, n_j\geq 1} \frac{1}{\prod_{j=1}^{\ell} \Gamma(\alpha n_j + 1)},$$

providing a closed form and thereby avoiding recurrence relations.

Obviously, for $\alpha = 1$, we have that (21) is the inverse of the usual matrix exponential:

Theorem 2. *Let* $A \in \mathbb{C}^{r\times r}$ *be a square matrix and* $\alpha = 1$*. Then, the matrix sequence defined by* (20) *satisfies*

$$D_n(1) = \frac{(-1)^n A^n}{n!}, \quad n \geq 0. \tag{22}$$

Proof of Theorem 2. We proceed by mathematical induction on. For $\alpha = 1$, from definition (20), one obtains for the base case ($n = 0$):

$$D_0(1) = I_{r\times r} = \frac{(-1)^0 A^0}{0!}.$$

In the same way, taking $n = 1$, the definition of sequence $D_n(1)$ immediately yields

$$D_1(1) = -\frac{AD_0(1)}{1!} = -\frac{A}{1!} = \frac{(-1)^1 A^1}{1!}.$$

Finally, in the induction step, we suppose that for $k = 0, 1, 2, \ldots, n-1$, property (22) is true. Then, for n, we conclude

$$\begin{aligned} D_n(1) &= -\sum_{k=0}^{n-1} \frac{A^{n-k} D_k(1)}{(n-k)!} = -\sum_{k=0}^{n-1} \frac{A^{n-k}(-1)^k A^k}{(n-k)!k!} = -\frac{A^n}{n!} \sum_{k=0}^{n-1} \frac{(-1)^k n!}{(n-k)!k!} = -\frac{A^n}{n!} \sum_{k=0}^{n-1} \binom{n}{k} (-1)^k \\ &= -\frac{A^n}{n!} \left[\sum_{k=0}^{n} \binom{n}{k} (-1)^k - \binom{n}{n} (-1)^n \right] = -\frac{A^n}{n!} \left[-\binom{n}{n} (-1)^n \right] = \frac{(-1)^n A^n}{n!}. \end{aligned}$$

□

Now, we move on to the numerical computation of the inverse of the Caputo matrix exponential evaluated in the previous example.

Example 2. *In Example 1, we have shown that the matrix inverse of the Caputo matrix exponential* $\exp_\star(t^\alpha A; \alpha)$ *for* $A = \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}$ *and* $\alpha = 1/4$ *exists at least for t within the interval* $I = [0, 0.0000594]$*. It is easy to verify that* $t = 4 \times 10^{-5} \in I$ *produces the following numerical result*

$$\exp_\star\left(\left(4\times 10^{-5}\right)^{1/4} \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; 1/4 \right) = \begin{pmatrix} 1.177537946538906 & -0.08207192162719279 \\ 0.32828768650877116 & 0.767178338402942 \end{pmatrix},$$

and then

$$\exp_\star\left(\left(4\times 10^{-5}\right)^{1/4} \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; 1/4 \right)^{-1} = \begin{pmatrix} 0.8246349372113879 & 0.08821856737867267 \\ -0.3528742695146907 & 1.2657277741047512 \end{pmatrix}.$$

Evaluating only the first 13 terms of the series (21) with $f(0.00004, 0.25)$, we obtain

$$f_{13}(4\times 10^{-5}, 1/4) = \sum_{k=0}^{13} D_k(1/4)(4\times 10^{-5})^{k/4} = \begin{pmatrix} 0.8246349372113879 & 0.08821856737867273 \\ -0.3528742695146909 & 1.2657277741047515 \end{pmatrix},$$

with an approximation error

$$\left\| \exp_\star\left(\left(4\times 10^{-5}\right)^{1/4} \begin{pmatrix} 2 & -1 \\ 4 & -3 \end{pmatrix}; 1/4\right)^{-1} - f_{13}(4\times 10^{-5}, 1/4) \right\|_2 = 3.1650\times 10^{-16}.$$

Example 3. *Consider again the matrix A given in (13). In this case, the elements of the matrix sequence $\{D_n(\alpha)\}_{n\geq 0}$ can be calculated explicitly:*

$$\begin{aligned} D_0(\alpha) &= I_{4\times 4}, \\ D_1(\alpha) &= -\frac{A}{\Gamma(\alpha+1)}, \\ D_2(\alpha) &= A^2\left(\frac{1}{\Gamma(\alpha+1)^2} - \frac{1}{\Gamma(2\alpha+1)}\right), \\ D_3(\alpha) &= A^3\left(-\frac{1}{\Gamma(\alpha+1)^3} + \frac{2}{\Gamma(2\alpha+1)\Gamma(\alpha+1)} - \frac{1}{\Gamma(3\alpha+1)}\right), \\ D_n(\alpha) &= 0 \quad \text{for} \quad n\geq 4. \end{aligned}$$

Taking into account Definition (21), one simplifies

$$\begin{aligned} f(t,\alpha) &= \sum_{n\geq 0} D_n(\alpha)t^{n\alpha} = \sum_{n=0}^{3} D_n(\alpha)t^{n\alpha} = D_0(\alpha) + D_1(\alpha)t^{\alpha} + D_2(\alpha)t^{2\alpha} + D_3(\alpha)t^{3\alpha} \\ &= I_{4\times 4} - \frac{A}{\Gamma(\alpha+1)}t^{\alpha} + A^2\left(\frac{1}{\Gamma(\alpha+1)^2} - \frac{1}{\Gamma(2\alpha+1)}\right)t^{2\alpha} \\ &\quad + A^3\left(-\frac{1}{\Gamma(\alpha+1)^3} + \frac{2}{\Gamma(2\alpha+1)\Gamma(\alpha+1)} - \frac{1}{\Gamma(3\alpha+1)}\right)t^{3\alpha} \\ &= \begin{pmatrix} 1 & -\frac{t^{\alpha}}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(\alpha+1)^2} - \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} & -\frac{t^{3\alpha}}{\Gamma(\alpha+1)^3} + \frac{2t^{3\alpha}}{\Gamma(\alpha+1)\Gamma(2\alpha+1)} - \frac{t^{3\alpha}}{\Gamma(3\alpha+1)} \\ 0 & 1 & -\frac{t^{\alpha}}{\Gamma(\alpha+1)} & \frac{t^{2\alpha}}{\Gamma(\alpha+1)^2} - \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} \\ 0 & 0 & 1 & -\frac{t^{\alpha}}{\Gamma(\alpha+1)} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \end{aligned}$$

which gives the same result as the matrix inverse already calculated in (14).

5. Conclusions

The starting point of this discussion was the observation and well-known fact that the conventional matrix exponential always possesses an inverse due to its semigroup property. On the other hand, Caputo's matrix exponential carries a leading role in fractional calculus.

In this work, we have shown that for the Caputo matrix exponential the inverse does not necessarily exist per se. Nevertheless, its existence is guaranteed in a specific interval, which we have determined to relate to an uncomplicated inequality, viz. Equation (12). Furthermore, we have established that this inverse is generally not again a Caputo matrix exponential.

Additionally, several explicit procedures have been outlined to calculate the inverse of the Caputo matrix exponential, and it is hoped that they will open up novel pathways for the development of future numerical methods for its efficient computation.

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