Highly Accurate Global Padé Approximations of Generalized Mittag-Leffler Function and its Inverse

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Abstract

The two-parametric Mittag-Leffler function (MLF), $E_{\alpha,\beta}$, is fundamental to the study and simulation of fractional differential and integral equations. However, these functions are computationally expensive and their numerical implementations are challenging. In this paper, we present a unified framework for developing global rational approximants of $E_{\alpha,\beta}(-x)$, x > 0, with $\{(\alpha,\beta) : 0 < \alpha \leq 1, \beta \geq \alpha, (\alpha,\beta) \neq (1,1)\}$. This framework is based on the series definition and the asymptotic expansion at infinity. In particular, we develop three types of fourth-order global rational approximations and discuss how they could be used to approximate the inverse function. Unlike existing approximations which are either limited to MLF of one parameter or of low accuracy for the two-parametric MLF, our rational approximants are of fourth order accuracy and have low percentage error globally. For efficient utilization, we study the partial fraction decomposition and use them to approximate the two-parametric MLF with a matrix argument which arise in the solutions of fractional evolution differential and integral equations.

Keywords: Mittag-Leffler functions; Fractional evolution equations; Rational approximation; Global Padé approximation; Matrix function

1. Introduction

In this paper, we consider the two-parametric MLF

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \qquad \operatorname{Re} \alpha > 0, \quad \beta \in \mathbb{C}, \quad z \in \mathbb{C}.$$
(1)

This entire function generalizes the MLF of one-parameter, $E_{\alpha} = E_{\alpha,1}$.

The function $E_{\alpha,\beta}$ plays a key role in the study and simulation of history-dependent evolution models that arise in many engineering and science areas such as flow in porous media, pattern recognition, rheology, anomalous diffusion, electric networks, etc. In particular, it is the cornerstone of the development of generalized exponential time differencing (GETD) schemes [7] which extend the notion of exponential integrator [19] to time-fractional problems. Evaluation of $E_{\alpha,\beta}$ with scalar arguments is very expensive and challenging. Although the series (1) converges analytically for all $z \in \mathbb{C}$, it is not practical or may not be valid to use it computationally for $|z| \geq 1$. Consequently, different techniques for the evaluation of $E_{\alpha,\beta}$ have been developed. Gorenflo, Loutchko and Luchko [11] proposed an algorithm based on using appropriate techniques for different regions of \mathbb{C} . For small and large |z| values, they used the series definition (1) and the asymptotic series at infinity, respectively. For the intermediate regions they used the integral representations. A similar approach has been followed by Hilfer and Seybold [13]. Garrappa [8] provided an approach based on the numerical inversion of the Laplace transform. For efficient implementation, he provided an algorithm for finding the optimal parabolic contour on the basis of the distance and strength of the singularities of the Laplace transform.

The evaluation of MLF with a matrix argument is still a tricky and tough task. Garrappa [9] developed an algorithm based on the similarity transform. This approach requires the evaluation of MLF and its derivatives for each eigenvalue, which is again obtained using the Laplace transform. Clearly, massive calculations will be required for large full matrices.

In summary, all existing algorithms for evaluating $E_{\alpha,\beta}$ suffer from some drawbacks such as nontrivial software implementation, long CPU time especially when a fine error tolerance is imposed, overflow numbers, and catastrophic cancellations. Due to these computational complexities and the need for efficient matrix function evaluation, accurate and efficient approximations are imperative.

To the best of authors' knowledge, there have been few studies about rational approximations of MLF. Freed *et al.* [5] developed a piecewise approximant for $E_{\alpha}(-x^{\alpha})$, x > 0, based on the truncated series representation for small values, the asymptotic expansion for large values, and a Padé type approximant for the intermediate values. For $E_{\alpha}(-x)$, x > 0, Starovoitov and Starovoitova [23] analyzed Padé type approximants of the form p_n/q_m , $m \leq n$, and discussed their asymptotic rate of convergence on the compact unit disk as $n \to \infty$. Borhanifar and Valizadeh [3] constructed a fourth order Padé approximant and used it to develop a numerical scheme for the time-space diffusion equation. Iyiola *et al.* [15] constructed a second order non-Padé type rational approximation for $E_{\alpha,\beta}$ using real distinct poles (RDP). However, although the approximants in [3] and [15] might be adequate for small values, they fail to account for the asymptotic power law behavior.

The global Padé approximation technique introduced by Winitzki [24] has been applied recently to construct rational approximations for the Mittag-Leffler function and its generalization. In this technique, rational approximations are constructed by matching them with selected combinations of the series definition and the asymptotic expansion. Atkinson and Osseiran [1] used this technique to construct a second-order rational approximation for E_{α} . Later, Ingo *et al.* [14] showed that the rational approximant in [1] is not satisfactory for α close to one. Alternatively, they constructed a fourth-order global approximation for E_{α} that behaves reasonably well for all values of $\alpha \in (0, 1)$. Zeng [25] extended this technique to construct a second-order global Padé approximant for $E_{\alpha,\beta}$. However, this approximation is not satisfactory for α close to one, especially when $\beta = 1$ and it is malfunctioning for $\beta = \alpha$, $0.5 \leq \alpha < 1$.

As for the inverse of MLF, Hilfer and Seybold [13] introduced the inverse of $E_{\alpha,\beta}(z)$ as the solution of the equation

$$L_{\alpha,\beta}(E_{\alpha,\beta}(z)) = z, \qquad z \in \mathbb{C},$$
(2)

where $L_{\alpha,\beta}(z)$ is evaluated by solving the functional equation (2) numerically. They

discussed the principal branch of the function and showed that it reduces to the principal branch of the logarithm function as $\alpha \to 1$ when $\beta = 1$. Hanneken and Achar [12] proposed a finite series representation for $L_{\alpha,\beta}$ but only for some values of $\alpha \in (0, \frac{1}{2})$ and $\beta = 1, 2$. Lately, approximations of $L_{\alpha,\beta}$ have been introduced to overcome the difficulty of solving the functional equation (2). Atkinson and Osseiran [1]; and Ingo *et al.* [14] discussed the approximation of $(-L_{\alpha,1})$ based on the inversion of their global Padé approximants. Similarly, Zeng and Chen [25]; and Iyiola *et al.* [15] inverted their second order approximants of $E_{\alpha,\beta}$ to obtain an approximation of $(-L_{\alpha,\beta})$.

Consequently, based on the current state of the literature, more accurate rational approximations of $E_{\alpha,\beta}$ and its inverse are needed. Such approximations are expected to ease computation cost and yield accurate values globally. In this paper, we introduce a framework that unifies the notion of global Padé approximation for the two-parametric MLF. Moreover, we develop different types of fourth-order global rational approximations for $E_{\alpha,\beta}(-x)$, x > 0, for $\{(\alpha,\beta): 0 < \alpha \leq 1, \beta \geq \alpha, (\alpha,\beta) \neq (1,1)\}$. We also discuss analytically and numerically the approximation errors. Furthermore, we present the partial fraction decomposition of the rational approximants together with its advantage in efficient implementation for matrix arguments. An algorithm for computing $(-L_{\alpha,\beta})$ based on the inversion of our fourth order approximants is presented. All along, we demonstrate through numerical experiments and comparisons, that the new developed fourth-order approximants provide superior global approximations for $E_{\alpha,\beta}$ and its special case E_{α} .

This paper is organized as follows. Section 2 contains the unified framework for the global Padé approximation and the error analysis. In section 3, we discuss the second order global Padé approximant constructed by Zeng and Chen in [25] and the need for more accurate approximants. Section 4 contains the construction of our fourth order approximants. The partial fraction decomposition and the algorithms to compute the poles and weights are discussed in section 5. In section 6 we discuss the inverse MLF and its approximation through the inversion of our rational approximants. Graphical and numerical demonstrations of the performance of our approximants are presented in section 7. In section 8, we apply our approximants to the solutions of fractional differential and integral equations and systems.

The computations in this paper are performed using Matlab software on a dell laptop with a core i5 processor.

2. Global rational approximation for $E_{\alpha,\beta}(-x), x > 0$

In this section, we introduce and outline the construction of the global Padé approximation for $E_{\alpha,\beta}(-x)$, x > 0, for the cases

$$\mathcal{A} = \{ (\alpha, \beta) : 0 < \alpha \le 1, \beta \ge \alpha, (\alpha, \beta) \ne (1, 1) \}.$$
(3)

Our approach is based on the technique proposed by Winitzki in [24]. This technique relies on the asymptotic expansion given by the following theorem ([20], Theorem 1.4).

Theorem 2.1. Let $\alpha \in (0,2)$, $\beta \in \mathbb{C}$ and $\mu \in \mathbb{R}$, $\frac{\pi \alpha}{2} < \mu < \min\{\pi, \pi \alpha\}$. Then for $\mu \leq |\arg z| \leq \pi$,

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{n} \frac{(z)^{-k}}{\Gamma(\beta - \alpha k)} + \mathcal{O}(|z|^{-(n+1)}), \quad as \ |z| \to \infty, \quad n \ge 1.$$
(4)

In particular, when $\beta = \alpha$, the series in (4) takes the form

$$E_{\alpha,\alpha}(z) = -\sum_{k=1}^{n-1} \frac{z^{-(k+1)}}{\Gamma(-\alpha k)} + \mathcal{O}(|z|^{-(n+1)}), \quad \text{as } |z| \to \infty, \quad n \ge 2.$$
(5)

As an abbreviation for the rest of the paper, the cases $\beta > \alpha$ and $\beta = \alpha$ are to be understood as sub-cases of (3).

2.1. Definition

We proceed by considering the function

$$\mathcal{E}_{\alpha,\beta}(x) = s_{\alpha,\beta}(x) E_{\alpha,\beta}(-x),\tag{6}$$

with $s_{\alpha,\beta}(x)$ chosen so that the first term in the asymptotic expansion of $\mathcal{E}_{\alpha,\beta}$ is 1. It follows from (4) and (5) that

$$s_{\alpha,\beta}(x) = \begin{cases} \Gamma(\beta - \alpha)x, & \beta > \alpha, \\ \\ -\Gamma(-\alpha)x^2, & \beta = \alpha. \end{cases}$$
(7)

This function admits the following behavior:

$$\mathcal{E}_{\alpha,\beta}(x) = \begin{cases} a(x) + \mathcal{O}(x^m), & \text{as } x \to 0, \quad m \ge \begin{cases} 2, & \beta > \alpha, \\ 3, & \beta = \alpha, \end{cases} \\ b(x^{-1}) + \mathcal{O}(x^{-n}), & \text{as } x \to \infty, \quad n \ge \begin{cases} 1, & \beta > \alpha, \\ 2, & \beta = \alpha, \end{cases} \end{cases}$$
(8)

where, from (1),

$$a(x) = \begin{cases} \Gamma(\beta - \alpha) x \sum_{k=0}^{m-2} \frac{(-x)^k}{\Gamma(\beta + \alpha k)}, & \beta > \alpha, \\ \\ -\Gamma(-\alpha) x^2 \sum_{k=0}^{m-3} \frac{(-x)^k}{\Gamma(\alpha k + \alpha)}, & \beta = \alpha, \end{cases}$$
(9)

and from (4)-(5),

$$b(x^{-1}) = \begin{cases} -\Gamma(\beta - \alpha) x \sum_{k=1}^{n} \frac{(-x)^{-k}}{\Gamma(\beta - \alpha k)}, & \beta > \alpha, \\ \\ \Gamma(-\alpha) x^{2} \sum_{k=1}^{n} \frac{(-x)^{-(k+1)}}{\Gamma(-\alpha k)}, & \beta = \alpha. \end{cases}$$
(10)

Note that when n = 1, then $b(x^{-1}) = 1$. We will see later (equation (18)) that in this case the asymptotic expansion in (8) does not contribute to the rational approximation of $\mathcal{E}_{\alpha,\beta}$. Therefore, for our purposes, we always take n > 1.

Next, we introduce the following definition.

Definition 2.2. Consider $E_{\alpha,\beta}$ with $(\alpha,\beta) \in \mathcal{A}$. Let m and n be positive integers such that

$$n > 1, \qquad m \ge \begin{cases} 2, & \text{if } \beta > \alpha, \\ 3, & \text{if } \beta = \alpha, \end{cases}, \qquad m + n \text{ is odd.}$$
(11)

Then, the global Padé approximation, $R^{m,n}_{\alpha,\beta}(x)$, of type (m,n) for $E_{\alpha,\beta}(-x)$ is defined as

$$R^{m,n}_{\alpha,\beta}(x) = \frac{1}{s_{\alpha,\beta}(x)} \frac{p(x)}{q(x)}, \quad 0 < \alpha \le 1, \quad \beta \ge \alpha, \quad (\alpha,\beta) \ne (1,1), \tag{12}$$

where p and q are polynomials of degree ν ,

$$\nu := \frac{m+n-1}{2} \ge 1,$$
(13)

such that $q(x) \neq 0$ for x > 0 and

$$\frac{p(x)}{q(x)} = \begin{cases} a(x) + \mathcal{O}(x^{m-\nu}), & \text{as } x \to 0, \\ \\ b(x^{-1}) + \mathcal{O}(x^{-n}), & \text{as } x \to \infty. \end{cases}$$
(14)

Next, we present the procedure for constructing $R^{m,n}_{\alpha,\beta}(x)$.

2.2. Construction of $R^{m,n}_{\alpha,\beta}(x)$

Let m and n be as in (11). We seek a rational approximation of the form

$$\mathcal{E}_{\alpha,\beta}(x) \approx \frac{p(x)}{q(x)} = \frac{p_0 + p_1 x + \dots + p_\nu x^\nu}{q_0 + q_1 x + \dots + q_\nu x^\nu},$$
(15)

where ν is as in (13). This means that $2\nu + 1$ coefficients are to be determined.

Since $\mathcal{E}_{\alpha,\beta}(x) \to 1$ as $x \to \infty$ and $\lim_{x\to\infty} p(x)/q(x) = p_{\nu}/q_{\nu}$, we can set

$$p_{\nu} = q_{\nu} = 1$$

To find the other 2ν unknowns $\{p_i, q_i\}_{i=0}^{\nu-1}$, we solve the system of linear equations obtained by satisfying the requirement (14) which takes the form

$$p(x) - q(x)a(x) = \mathcal{O}(x^m), \qquad \text{as } x \to 0, \qquad (16)$$

$$x^{-\nu}p(x) - x^{-\nu}q(x)b(x^{-1}) = \mathcal{O}(x^{-n}),$$
 as $x \to \infty.$ (17)

By expanding the left-hand side of (16), it follows that the coefficients of x^k , $k = 0, 1, \ldots, m - 1$, must vanish. As such, we obtain m linear equations. Similarly, by expanding the left hand side of (17), the coefficients of

$$x^{-1}, x^{-2}, \dots, x^{-(n-1)}$$
 (18)

must vanish and we obtain another system of n-1 linear equations. Collectively, (16) and (17) yield a linear system of m+n-1 (= 2ν) equations which are then solved for the 2ν unknowns. By inspection, we have

$$\begin{cases} p_0 = 0, & \beta > \alpha, \\ p_0 = p_1 = 0, & \beta = \alpha. \end{cases}$$
(19)

Hence, for $\beta > \alpha$ we solve $2\nu - 1$ (= m + n - 2) equations with m + n - 2 unknowns, while for $\beta = \alpha$ we solve $2\nu - 2$ (= m + n - 3) equations with m + n - 3 unknowns.

We will see later (Remark 2.3) that for controlling the approximation error we must have m > n. Table (1) provides the order of approximations for the types (m, n) with m > n > 1 and m + n is odd.

| $n \atop m$ | 2 | 3 | 4 | 5 |
|----------------------------|-------------|-----------------------|-------------|--------|
| 3 4 5 6 7 8 | 2 3 4 | 3 • 4 • 5 | 4 • 5 | 5 6 |

Table 1: Order of approximations for different types (m, n)

2.3. Approximation error

Consider the pointwise error

$$e_{\alpha,\beta}^{m,n}(x) := E_{\alpha,\beta}(-x) - R_{\alpha,\beta}^{m,n}(x), \qquad x > 0.$$
 (20)

Equations (6), (7), (8), (12), and (14) yield the following orders. As $x \to 0$, we have

$$e_{\alpha,\beta}^{m,n}(x) = E_{\alpha,\beta}(-x) - R_{\alpha,\beta}^{m,n}(x) = \frac{1}{s_{\alpha,\beta}(x)} \left\{ \mathcal{E}_{\alpha,\beta}(x) - \frac{p(x)}{q(x)} \right\}$$
$$= \frac{1}{s_{\alpha,\beta}(x)} \left\{ a(x) + \mathcal{O}(x^m) - a(x) - \mathcal{O}(x^{m-\nu}) \right\}$$
$$= \frac{1}{s_{\alpha,\beta}(x)} \left\{ \mathcal{O}(x^m) + \mathcal{O}(x^{m-\nu}) \right\}$$
$$= \left\{ \begin{array}{l} \mathcal{O}(x^{m-\nu-1}), & \beta > \alpha, \\ \mathcal{O}(x^{m-\nu-2}), & \beta = \alpha. \end{array} \right.$$
(21)

As $x \to \infty$, we have

$$e_{\alpha,\beta}^{m,n}(x) = E_{\alpha,\beta}(-x) - R_{\alpha,\beta}^{m,n}(x) = \frac{1}{s_{\alpha,\beta}(x)} \left\{ \mathcal{E}_{\alpha,\beta}(x) - \frac{p(x)}{q(x)} \right\}$$
$$= \frac{1}{s_{\alpha,\beta}(x)} \left\{ b(x^{-1}) + \mathcal{O}(x^{-n}) - b(x^{-1}) - \mathcal{O}(x^{-n}) \right\}$$
$$= \frac{1}{s_{\alpha,\beta}(x)} \mathcal{O}(x^{-n})$$

$$=\begin{cases} \mathcal{O}(x^{-n-1}), & n > 1, \quad \beta > \alpha, \\ \mathcal{O}(x^{-n-2}), & n > 1, \quad \beta = \alpha. \end{cases}$$
(22)

Remark 2.3. By inspection of (21) and (22), one can observe the following.

• For reliable approximations of $R^{m,n}_{\alpha,\beta}$ at small values, one should consider $m \ge n+1$ when $\beta \ne \alpha$ and $m \ge n+3$ when $\beta = \alpha$. This is why, for example, $R^{5,4}_{\alpha,\beta}$ is not a good approximation when $\beta = \alpha$. • For large values of x, the approximation error can be made arbitrary small by taking n sufficiently large. However, this may not be the case since the asymptotic series (4) of the Mittag-Leffler function is divergent.

Remark 2.4. In all the numerical experiments and comparisons throughout this paper, the term "exact" values of MLF refers to the values computed using the routines discussed in [8] and [9].

3. Second-order global Padé approximant $R^{3,2}_{\alpha,\beta}$

For completeness, we provide here an overview of the second order global Padé approximant $R^{3,2}_{\alpha,\beta}(x)$ constructed by Zeng and Chen in [25]. The approximant is given by

$$R^{3,2}_{\alpha,\beta}(x) = \frac{1}{\Gamma(\beta - \alpha)} \frac{p_1 + x}{q_0 + q_1 x + x^2}, \qquad \beta > \alpha,$$
(23)

with

$$p_{1} = c_{\alpha,\beta} \left[\Gamma(\beta)\Gamma(\beta + \alpha) - \frac{\Gamma(\beta + \alpha)\Gamma^{2}(\beta - \alpha)}{\Gamma(\beta - 2\alpha)} \right],$$

$$q_{0} = c_{\alpha,\beta} \left[\frac{\Gamma^{2}(\beta)\Gamma(\beta + \alpha)}{\Gamma(\beta - \alpha)} - \frac{\Gamma(\beta)\Gamma(\beta + \alpha)\Gamma(\beta - \alpha)}{\Gamma(\beta - 2\alpha)} \right],$$

$$q_{1} = c_{\alpha,\beta} \left[\Gamma(\beta)\Gamma(\beta + \alpha) - \frac{\Gamma^{2}(\beta)\Gamma(\beta - \alpha)}{\Gamma(\beta - 2\alpha)} \right],$$

$$c_{\alpha,\beta} = \frac{1}{\Gamma(\beta + \alpha)\Gamma(\beta - \alpha) - \Gamma^{2}(\beta)},$$
(24)

and

$$R^{3,2}_{\alpha,\alpha}(x) = \frac{\alpha}{\Gamma(1+\alpha) + \frac{2\Gamma(1-\alpha)^2}{\Gamma(1-2\alpha)}x + \Gamma(1-\alpha)x^2}, \qquad 0 < \alpha < 1.$$
(25)

As shown in Figures 1 and 2, the approximation $R^{3,2}_{\alpha,\beta}$ could be reasonable for small values of α , however, it is not adequate otherwise.

4. Fourth-order global Padé approximants

Fourth order global Padé approximants ($\nu = 4$) correspond to the types (m, n) with m + n = 9. They include the types (5, 4), (6, 3), and (7, 2). As discussed in subsection 2.2, the approximation $R_{\alpha,\beta}^{m,n}$ for $\nu = 4$ takes the form

$$R_{\alpha,\beta}^{m,n}(x) = \begin{cases} \frac{1}{\Gamma(\beta-\alpha)} \frac{p_1 + p_2 x + p_3 x^2 + x^3}{q_0 + q_1 x + q_2 x^2 + q_3 x^3 + x^4}, & \beta > \alpha, \\ \frac{-1}{\Gamma(-\alpha)} \frac{\hat{p}_2 + \hat{p}_3 x + x^2}{\hat{q}_0 + \hat{q}_1 x + \hat{q}_2 x^2 + \hat{q}_3 x^3 + x^4}, & \beta = \alpha. \end{cases}$$
(26)

The unknown coefficients are obtained by applying (16) and (17). Below we present the systems for these coefficients for the different types.



Figure 1: Plots of $R^{3,2}_{\alpha,1}$ for different values of α



Figure 2: Plots of $R^{3,2}_{\alpha,\beta}$ for $\beta = \alpha = 0.25$ (left) and $\beta = \alpha = 0.5$ (right)

4.1. Coefficients of $R^{5,4}_{\alpha,\beta}$ For $\beta > \alpha$, the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 \\ 0 & 0 & 1 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 \\ 0 & 0 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-3\alpha)} \\ 1 & 0 & 0 & 0 & -1 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-3\alpha)} \\ 0 & 1 & 0 & 0 & 0 & -1 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-\alpha)} \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \end{pmatrix}$$

$$(27)$$

For $\beta = \alpha$ the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0 & 0 \\ 0 & 1 & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0 \\ 0 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 \\ 0 & 0 & 0 & -1 & -\frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} & 0 \\ 1 & 0 & 0 & 0 & -1 & \frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} \\ 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} \hat{p}_2 \\ \hat{p}_3 \\ \hat{q}_0 \\ \hat{q}_1 \\ \hat{q}_2 \\ \hat{q}_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \\ 0 \\ -\frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} \end{pmatrix}.$$
(28)

4.2. Coefficients of $R^{6,3}_{\alpha,\beta}$

For $\beta > \alpha$, the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 \\ 0 & 0 & 1 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 \\ 0 & 0 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} \\ 0 & 0 & 0 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+4\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} \\ 0 & 1 & 0 & 0 & 0 & -1 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-\alpha)} \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \end{pmatrix},$$

(29)

For $\beta = \alpha$, the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0 & 0 \\ 0 & 1 & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0 \\ 0 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 \\ 0 & 0 & -\frac{\Gamma(-\alpha)}{\Gamma(4\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} \\ 1 & 0 & 0 & 0 & -1 & \frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} \\ 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{pmatrix} \hat{p}_2 \\ \hat{p}_3 \\ \hat{q}_0 \\ \hat{q}_1 \\ \hat{q}_2 \\ \hat{q}_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \\ \frac{\Gamma(-\alpha)}{\Gamma(-3\alpha)} \\ -\frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} \end{pmatrix}.$$
(30)

4.3. Coefficients of $R^{7,2}_{\alpha,\beta}$

For $\beta > \alpha$, the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 & 0 \\ 0 & 0 & 1 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} & 0 \\ 0 & 0 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta)} \\ 0 & 0 & 0 & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+4\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} \\ 0 & 0 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+5\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+4\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+4\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} \\ 0 & 0 & 0 & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+5\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+4\alpha)} & \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+3\alpha)} & -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta+2\alpha)} \\ \end{bmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ q_0 \\ q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ \frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-\alpha)} \\ -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-\alpha)} \\ -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \\ -\frac{\Gamma(\beta-\alpha)}{\Gamma(\beta-2\alpha)} \end{pmatrix}$$

For $\beta = \alpha$, the coefficients satisfy the system

$$\begin{bmatrix} 1 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0 & 0\\ 0 & 1 & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0 & 0\\ 0 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(\alpha)} & 0\\ 0 & 0 & -\frac{\Gamma(-\alpha)}{\Gamma(4\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(\alpha)}\\ 0 & 0 & \frac{\Gamma(-\alpha)}{\Gamma(5\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(4\alpha)} & \frac{\Gamma(-\alpha)}{\Gamma(3\alpha)} & -\frac{\Gamma(-\alpha)}{\Gamma(2\alpha)}\\ 0 & 1 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \hat{p}_2\\ \hat{p}_3\\ \hat{q}_0\\ \hat{q}_1\\ \hat{q}_2\\ \hat{q}_3 \end{bmatrix} = \begin{pmatrix} 0\\ 0\\ -1\\ 0\\ \frac{\Gamma(-\alpha)}{\Gamma(-3\alpha)}\\ -\frac{\Gamma(-\alpha)}{\Gamma(-2\alpha)} \end{pmatrix}.$$
(32)

Remark 4.1. Although the type (m, n) of the fourth order global Padé approximant of $E_{\alpha}(-x)$ by Ingo et al. [14] is not given, based on their construction, we expect the type to be a special case of one of the approximants above when $\beta = 1$.

5. Partial fraction decomposition

Partial fraction decomposition provides an efficient form for evaluating rational functions. In a recent work by [2], the efficiency of using partial fraction decomposition for computing functions of matrices is discussed. This efficiency is indisputable when the poles are complex conjugates and the argument is a matrix.

Unlike the Padé approximations for the exponential function, the poles of $R^{m,n}_{\alpha,\beta}$ are functions of α and β . Fortunately, through direct calculations, one can show that for most $(\alpha, \beta) \in \mathcal{A}$, the poles of $R^{m,n}_{\alpha,\beta}$ are complex conjugates. Next, we explore the partial fraction decomposition of these approximations.

5.1. Decomposition of second-order global Padé approximant

The second-order global Padé approximant $R^{3,2}_{\alpha,\beta}$ admits the partial fraction decomposition

$$R^{3,2}_{\alpha,\beta}(x) = \frac{c_1}{x - r_1} + \frac{c_2}{x - r_2},$$

where

$$r_1 = \frac{-q_1 + \sqrt{q_1^2 - 4q_0}}{2}, \qquad r_2 = \frac{-q_1 - \sqrt{q_1^2 - 4q_0}}{2},$$

and

$$c_1 = \frac{p_1 - r_1}{r_2 - r_1}, \qquad c_2 = \frac{p_1 - r_2}{r_1 - r_2}.$$

We can verify numerically that for $(\alpha, \beta) \in \mathcal{A}$ we have $q_1^2 - 4q_0 < 0$ which imply that $r_2 = \bar{r}_1$ and $c_2 = \bar{c}_1$. As a result, we can write

$$R^{3,2}_{\alpha,\beta}(x) = 2 \operatorname{Re}\left[\frac{c_1}{x - r_1}\right].$$
(33)

5.2. Decomposition of the fourth-order global Padé approximants

The partial fraction decomposition for $R^{m,n}_{\alpha,\beta}$, (m,n) = (5,4), (6,3), (7,2), takes the form

$$R^{m,n}_{\alpha,\beta}(x) = \frac{c_1}{x - r_1} + \frac{c_2}{x - r_2} + \frac{c_3}{x - r_3} + \frac{c_4}{x - r_4}.$$
(34)

Empirically, for $(\alpha, \beta) \in \mathcal{A}$, these poles are complex conjugates. If we let $r_3 = \bar{r}_1$, $r_4 = \bar{r}_2$, $c_3 = \bar{c}_1$, and $c_4 = \bar{c}_2$, then the partial fraction decomposition can be written as

$$R^{m,n}_{\alpha,\beta}(x) = 2\operatorname{Re}\left[\frac{c_1}{x-r_1}\right] + 2\operatorname{Re}\left[\frac{c_2}{x-r_2}\right].$$
(35)

Computing of the poles and weights is outlined in the following algorithm.

6. Inverse Mittag-Leffler Function

The invertibility of $E_{\alpha,\beta}(-x)$, x > 0, follows from the complete monotonicity property of $E_{\alpha,\beta}$. As shown in [10], this function is completely monotone if and only if $0 < \alpha \leq 1$ and $\beta \geq \alpha$. Since $E_{\alpha,\beta}(0) = 1/\Gamma(\beta)$ and $\lim_{x\to\infty} E_{\alpha,\beta}(-x) = 0$, then for $0 < \alpha \leq 1$ and $\beta \geq \alpha$, the inverse function $-L_{\alpha,\beta}$ of $E_{\alpha,\beta}(-x)$, x > 0, is the function

$$-L_{\alpha,\beta}: (0, 1/\Gamma(\beta)] \to [0, \infty),$$

Algorithm 1 Poles and weights for partial fraction decomposition of fourth-order $R^{m,n}_{\alpha,\beta}$

such that

$$-L_{\alpha,\beta}(x) = y \text{ iff } x = E_{\alpha,\beta}(-y).$$
(36)

The inverse function can be approximated by inverting the approximations $R^{m,n}_{\alpha,\beta}$ of $E_{\alpha,\beta}(-x)$,

$$E_{\alpha,\beta}(-x) \approx R_{\alpha,\beta}^{m,n} = \frac{1}{s_{\alpha,\beta}(x)} \frac{p(x)}{q(x)}.$$

This is equivalent to computing the positive root r^+ of the equation

$$s_{\alpha,\beta}(x)q(x)y - p(x) = 0, \qquad (37)$$

where $y = E_{\alpha,\beta}(-r^+)$. Zeng and Chen in [25] solved a quadratic equation of the form (37) for $R^{3,2}_{\alpha,\beta}(x)$ to obtain the approximation

$$-L_{\alpha,\beta}(y) \approx \frac{1}{2\Gamma(\beta-\alpha)y} - \frac{q_1}{2} + \sqrt{\left(\frac{q_1}{2} - \frac{1}{2\Gamma(\beta-\alpha)y}\right)^2 - q_0\left(1 - \frac{1}{\Gamma(\beta)y}\right)}, \quad \beta > \alpha,$$
(38)

and

$$-L_{\alpha,\alpha}(y) \approx -\frac{\Gamma(1-\alpha)}{\Gamma(1-2\alpha)y} + \sqrt{\frac{\Gamma^2(1-\alpha)}{\Gamma^2(1-2\alpha)y^2} - \frac{1+\alpha}{1-\alpha}\left(1-\frac{1}{\Gamma(\alpha)y}\right)}.$$
(39)

Approximating the inverse using our fourth order approximants involves finding the positive root of the fourth degree polynomial in (37), which takes the form

$$c_{\alpha,\beta} y q_0 - p_1 + (c_{\alpha,\beta} y q_1 - p_2) x + (c_{\alpha,\beta} y q_2 - p_3) x^2 + (c_{\alpha,\beta} y q_3 - 1) x^3 + c_{\alpha,\beta} y x^4 = 0, \quad c_{\alpha,\beta} = \Gamma(\beta - \alpha) \text{ for } \beta > \alpha, \quad (40)$$

$$c_{\alpha}y\hat{q}_{0} + \hat{p}_{2} + (c_{\alpha}y\hat{q}_{1} + \hat{p}_{3})x + (c_{\alpha}y\hat{q}_{2} + 1)x^{2} + c_{\alpha}y\hat{q}_{3}x^{3} + c_{\alpha}yx^{4} = 0, \quad c_{\alpha} = \Gamma(-\alpha) \text{ for } \beta = \alpha.$$
(41)

It is quite tedious to solve (40) and (41) analytically. Alternatively, the following algorithm can be employed. One can verify numerical that each of (40) and (41) has a unique positive root.

Algorithm 2 Approximation of the inverse MLF

Step 1 Specify m, n, α, β, y . Step 2 If $\beta > \alpha$ Compute the coefficient $c_{\alpha,\beta} = \Gamma(\beta - \alpha)$ Obtain p_i, q_i by solving the corresponding linear system. Find the roots of the polynomial (40) Then $-L_{\alpha,\beta}(y)$ is the unique positive root. If $\alpha = \beta$ Compute the coefficient $c_{\alpha} = \Gamma(-\alpha)$ Obtain \hat{p}_i, \hat{q}_i by solving the corresponding linear system. Find the roots of the polynomial (41)

Then
$$-L_{\alpha,\alpha}(y)$$
 is the unique positive root.

7. Performance and comparisons of the approximants

In this section, we demonstrate graphically and computationally the performance of the fourth-order global Padé approximants constructed above. We start by comparing the approximants $R_{\alpha,\beta}^{5,4}$, $R_{\alpha,\beta}^{6,3}$ and $R_{\alpha,\beta}^{7,2}$. Figures 3, 4 and 5 contain the profiles for different combinations of (α, β) . These profiles reveal that both $R_{\alpha,\beta}^{7,2}(x)$ and $R_{\alpha,\beta}^{6,3}(x)$ provide extremely well approximants and compare favorably with $R_{\alpha,\beta}^{5,4}(x)$. This observation supports our earlier argument in Remark 2.3 that approximations of the same order can be improved by increasing the number of local terms m and decreasing the number of asymptotic terms n in the matching requirements (16) and (17). The profile of the absolute errors are shown in Figure 6 and for completeness, we include in Figure 7 different profiles of $R_{\alpha,\beta}^{7,2}$ vs $R_{\alpha,\beta}^{3,2}$.

In table 2, we provide the maximum absolute error

$$\max_{x \in I} \{ |E_{\alpha,\beta}(-x) - R_{\alpha,\beta}(x)| \},\$$

and the maximum relative error

$$\max_{x \in I} \left\{ \left| \frac{E_{\alpha,\beta}(-x) - R_{\alpha,\beta}(x)}{E_{\alpha,\beta}(-x)} \right| \right\},\$$

where I is the interval [0, 10] and $R_{\alpha,\beta}$ is any of the approximants for $E_{\alpha,\beta}$. In the case $\beta = 1$, the errors resulting from $R_{\alpha,1}^{6,3}$ and $R_{\alpha,1}^{7,2}$ are smaller than those from the approximation by Ingo *et al.* in [14]. It is worth mentioning that they were comparing with "mlf" Matlab function by Podlubny which is based on the algorithm by Gorenflo *et al.* in [11] while we are comparing with the "ml" Matlab function by Garrappa [8].

Finally, in Figure 8 we compare the approximations of the inverse function obtained by solving (37) for $R_{\alpha,\beta}^{7,2}$ vs the exact values by definition (2).



Figure 3: Comparison of the fourth order approximants; $R_{\alpha,\beta}^{5,4}$, $R_{\alpha,\beta}^{6,3}$, $R_{\alpha,\beta}^{7,2}$ for $\beta = 1$



Figure 4: Comparison of the fourth order approximants; $R_{1,\beta}^{5,4}$, $R_{1,\beta}^{6,3}$, $R_{1,\beta}^{7,2}$ for $\beta = 1.01$ (left) and $\beta = 2$ (right)



Figure 5: Comparison of the fourth order approximants; $R_{\alpha,\alpha}^{5,4}$, $R_{\alpha,\alpha}^{6,3}$, $R_{\alpha,\alpha}^{7,2}$ for $\alpha = 0.5$ (left) and $\alpha = 0.75$ (right)



Figure 6: Plots of approximation errors $\left|e_{\alpha,\beta}^{m,n}(x)\right|$ for the fourth order approximants (7,2), (6,3), (5,4)



Figure 7: Comparisons of $R^{7,2}_{\alpha,\beta}$ and $R^{3,2}_{\alpha,\beta}$

| | $\alpha = 0.9$ | $, \beta = 1.9$ | $\alpha = 0.9$ | $\beta, \beta = 1$ | $\alpha = 0.5$ | $\beta = 0.5$ | $\alpha = 1.0$ | $\beta = 1.1$ | $\alpha = 1.0$ | $\beta = 2.0$ |
|--------------------------|----------------|-----------------|----------------|--------------------|----------------|---------------|----------------|---------------|----------------|---------------|
| | AE | RE | AE | RE | AE | RE | AE | RE | AE | RE |
| RDP | 0.0813 | 0.8234 | 0.1153 | 3.2415 | 0.0800 | 10.675 | 0.1225 | 3.3583 | 0.1165 | 1.165 |
| $R^{3,2}_{\alpha,\beta}$ | 0.0254 | 0.0526 | 0.1926 | 0.4884 | 0.1349 | 0.4697 | 0.3112 | 0.6394 | 0.0352 | 0.0755 |
| $R^{5,4}_{\alpha,\beta}$ | 0.0018 | 0.0052 | 0.0264 | 0.1552 | 0.0040 | 0.0119 | 0.1020 | 0.4274 | 0.0040 | 0.0119 |
| $R^{6,3}_{lpha,eta}$ | 0.0007 | 0.0034 | 0.0047 | 0.0920 | 0.0002 | 0.0028 | 0.0092 | 0.2278 | 0.0014 | 0.0073 |
| $R^{7,2}_{\alpha,\beta}$ | 0.0006 | 0.0055 | 0.0033 | 0.1648 | 0.0001 | 0.0033 | 0.0061 | 0.3949 | 0.0012 | 0.0112 |

Table 2: The maximum absolute error (AE) and maximum relative error (RE) for the different approximants

8. Applications

The fundamental importance of the two-parametric MLF and its inverse is the main motivation behind the construction of the approximants in this paper. Our objective here is to show the accuracy and efficiency of these approximants when applied to solutions of fractional differential and integral equations. The fourth order approximant $R_{\alpha,\beta}^{7,2}$ is used all through this section, while the second order approximant $R_{\alpha,\beta}^{3,2}$ is also applied for comparison purposes. Below, we consider some applications with solutions that involve MLF with scalar and matrix arguments.

8.1. Applications with scalar arguments

We start by considering the following applications that involve MLF with scalar arguments.

8.1.1. Fractional reaction-diffusion equation

Consider the following sub-diffusion initial-boundary value problem:

$$\begin{aligned} & ^{c} \partial_{t}^{\alpha} u(x,t) = u_{xx}(x,t) + u(x,t) \, u_{x}(x,t) + f(x,t), \quad x \in (0,1), t > 0, \\ & u(0,t) = u(1,t) = 0, \quad t \ge 0, \\ & u(x,0) = x(1-x), \qquad x \in [0,1], \end{aligned}$$
(42)

where ∂_t^{α} , $0 < \alpha < 1$, is the Caputo fractional derivative. When

$$f(x,t) = -\left[2 + E_{\alpha}(-t^{\alpha})(2x^{3} - 3x^{2} + x) + x(1-x)\right]E_{\alpha}(-t^{\alpha}),$$

then the exact solution is

$$u(x,t) = x(1-x)E_{\alpha}(-t^{\alpha}).$$
(43)

The solution profile and its approximations at x = 0.5 for $t \in [0, 10]$ and $\alpha = 0.5, 0.9$ are included in Figure 9. The corresponding errors and runtime (in seconds) for time increment of 0.01 are listed in Table 3 together with the runtime for ml subroutine in [9]. As can be observed, $R_{\alpha,\beta}^{7,2}$ provides an excellent approximation at a significantly reduced runtime as compared to the ml subroutine runtime. Furthermore, it is clear from the figures that, in general, $R_{\alpha,\beta}^{3,2}$ may not be a good option.



Figure 8: Plots of inverse MLF approximated by solving (37) for $R_{\alpha,\beta}^{7,2}$ vs the exact value obtained by applying the definition (2).



Figure 9: Plots of $R_{\alpha,\beta}^{7,2}$ and $R_{\alpha,\beta}^{3,2}$ approximations to the solution (43) of the fractional reactiondiffusion problem (42) at x = 0.5

| α | Max Abs. Error | Max Rel. Error | Runtime | ml Runtime |
|---|----------------|----------------|----------|------------|
| $\begin{array}{c} 0.5 \\ 0.9 \end{array}$ | 9.56e-06 | 6.77e-05 | 6.22e-04 | 7.25e-02 |
| | 8.25e-04 | 1.80e-03 | 7.06e-04 | 9.66e-02 |

Table 3: Errors and runtime for $R_{\alpha,\beta}^{7,2}$ approximation to the solution (43) of the fractional reactiondiffusion problem (42) at x = 0.5



Figure 10: Plots of $R_{\alpha,\beta}^{7,2}$ and $R_{\alpha,\beta}^{3,2}$ approximations to the solution (45) of the integral equation (44)

8.1.2. Fractional integral equation

Consider the following integral equation:

$$\mathcal{I}_{t}^{\alpha}u(t) + u(t) = t^{\beta-1}, \quad t > 0,$$
(44)

where α , $\beta > 0$ and \mathcal{I}^{α} is the Riemann-Liouville integral of order α . The exact solution of (44) is given by:

$$u(t) = \Gamma(\beta) t^{\beta - 1} E_{\alpha, \beta}(-t^{\alpha}).$$
(45)

Plots of the solution u(t) and its approximations for $(\alpha, \beta) = (0.6, 0.6)$ and (1.0, 1.5) are provided in Figure 10. The corresponding errors and runtime (in seconds) for time increment of 0.01 are listed in Table 4. Again, the results assert that superiority of $R_{\alpha,\beta}^{7,2}$.

| (α, β) | Max Abs. Error | Max Rel. Error | Runtime | ml Runtime |
|-------------------|----------------|----------------|----------|------------|
| (0.6, 0.6) | 3.77e-04 | 1.39e-04 | 3.00e-03 | 8.09e-02 |
| (1.0, 1.5) | 7.40e-03 | 8.70e-03 | 1.20e-03 | 1.09e-01 |

Table 4: Errors and runtime for $R^{7,2}_{\alpha,\beta}$ approximation to the solution (45) of the integral equation (44)

8.1.3. Ultraslow diffusion

The propagator p(x,t) of an ultraslow diffusive process satisfies the structural diffusion equation:

$$\frac{dp(x,t)}{d_m t} = k_\alpha \partial_x^2 p(x,t), \qquad t > 0, -\infty < x < \infty, \tag{46}$$



Figure 11: Plots of the propagator p(x,t) (47), of the ultraslow diffusion equation (46) together with the corresponding approximation using the inversion of $R_{\alpha,\beta}^{7,2}$ at x = 1 with $\alpha = 0.6$.

where the local structural derivative in time $\frac{dp(x,t)}{d_m t}$ with respect to the structural function E_{α}^{-1} is given by [17]

$$\frac{dp(x,t)}{d_m t} = \lim_{s \to t} \frac{p(x,s) - p(x,t)}{E_{\alpha}^{-1}(s) - E_{\alpha}^{-1}(t)}, \qquad 0 < \alpha < 1.$$

The solution of (46) (see [17]) is given by the scaled Gaussian function:

$$p(x,t) = \frac{1}{\sqrt{4\pi k_{\alpha} E_{\alpha}^{-1}(t)}} \exp\left(-\frac{x^2}{4k_{\alpha} E_{\alpha}^{-1}(t)}\right).$$
(47)

As shown in Figure 11, we have a good agreement between the propagator p(x,t) for $t \in (0,1)$, x = 1, and its approximation when E_{α}^{-1} is approximated by the inverse of $R_{\alpha,1}^{7,2}$.

8.2. Applications with matrix arguments

MLFs of matrix argument arise naturally in solutions of systems of fractional differential equations. The two-parametric MLF of a matrix $A \in \mathbb{C}^{n \times n}$ (see [22]) is given by:

$$E_{\alpha,\beta}(A) = \sum_{k=0}^{\infty} \frac{A^k}{\Gamma(\alpha k + \beta)}, \qquad \operatorname{Re} \alpha > 0, \quad \beta \in \mathbb{C}.$$
(48)

Next, we demonstrate the effectiveness of using $R_{\alpha,\beta}^{7,2}$ to approximate $E_{\alpha,\beta}$ of a matrix argument. The numerical experiments below show the runtime saving and accuracy in comparison with the ml_matrix function described in [9].

8.2.1. The Bagley-Torvik problem

The initial-value problem of Bagley-Torvik equation is given by

$$D^{2}u(t) + a_{1}{}^{c}D^{3/2}u(t) + a_{2}u(t) = f(t), \quad u(0) = 0, \ u'(0) = 0,$$
(49)

where a_1 and a_2 are positive constants. This problem models the motion of a thin, rigid plate immersed in a Newtonian fluid of infinite extension connected to a fixed point via a spring [16]. Using Laplace transform, the exact solution of (49) is

$$u(t) = \int_0^t G_{2,\frac{3}{2}}(t-\tau)f(\tau)d\tau,$$
(50)

where

$$G_{2,\frac{3}{2}}(t) = \sum_{n=0}^{\infty} \frac{(-a_2)^n}{n!} t^{2n+1} \Psi_1 \begin{bmatrix} (n+1,1) \\ (2n+2,\frac{1}{2}) \end{bmatrix} - a_1 t^{\frac{1}{2}} \end{bmatrix}.$$
 (51)

and $_{1}\Psi_{1}$ is the Wright function.

To avoid the complexity of calculating (51), using Theorem 8.1 in [4], the initial-value problem (49) can be converted into the system

$$D^{\frac{1}{2}}U(t) = AU(t) + f(t) e_4, \qquad U(0) = U^0,$$
(52)

where

$$U = \left(u, {}^{c}D^{\frac{1}{2}}u, {}^{c}D^{1}u, {}^{c}D^{\frac{3}{2}}u\right)^{T}, \quad e_{4} = (0, 0, 0, 1)^{T}, \qquad U^{0} = (0, 0, 0, 0)^{T}$$

and

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -a_2 & 0 & 0 & -a_1 \end{bmatrix}.$$

Then, the exact solution of (52) is [21]

$$U(t) = \int_0^t (t-\tau)^{-\frac{1}{2}} E_{\frac{1}{2},\frac{1}{2}}((t-\tau)^{\frac{1}{2}}A) e_4 f(\tau) d\tau.$$
(53)

For testing purposes, let

$$f(t) = a_2 t^2 + \frac{4a_1}{\sqrt{\pi}} t^{\frac{1}{2}} + 2.$$
(54)

Then the exact solution of (49) is

$$u(t) = t^2, (55)$$

while the solution (53) takes the form

$$U(t) = 2\left[t^{\frac{1}{2}}E_{\frac{1}{2},\frac{3}{2}}(At^{\frac{1}{2}}) + a_{1}tE_{\frac{1}{2},2}(At^{\frac{1}{2}}) + a_{2}t^{\frac{5}{2}}E_{\frac{1}{2},\frac{7}{2}}(At^{\frac{1}{2}})\right]e_{4}.$$
 (56)

Then the MLFs of matrix argument in (56) can be approximated using the partial fraction decomposition (35) of $R_{\alpha,\beta}^{7,2}$:

$$E_{\alpha,\beta}(B) \approx 2 \operatorname{Re} \left[c_1 (-B - Ir_1)^{-1} + c_2 (-B - Ir_2)^{-1} \right].$$

Explicitly, we have

$$2t^{\frac{1}{2}}E_{\frac{1}{2},\frac{3}{2}}(At^{\frac{1}{2}})e_{4} \approx 4\operatorname{Re}\left(t^{\frac{1}{2}}\left[c_{1}(-At^{\frac{1}{2}}-Ir_{1})^{-1}\right]e_{4}+t^{\frac{1}{2}}\left[c_{2}(-At^{\frac{1}{2}}-Ir_{2})^{-1}\right]e_{4}\right)$$
$$=4\operatorname{Re}[v_{1}+v_{2}],$$

where the vectors v_1 and v_2 are obtained by solving the systems

$$\left(-At^{\frac{1}{2}} - Ir_{1}\right)v_{1} = c_{1}t^{\frac{1}{2}}e_{4}, \qquad \left(-At^{\frac{1}{2}} - Ir_{2}\right)v_{2} = c_{2}t^{\frac{1}{2}}e_{4}$$

The remaining terms in (56) are approximated in a similar manner.

Figure 12 contains a comparison of the profiles of u and its approximation when $a_1 = 3$ and $a_2 = 1$. As can be observed, the partial fraction decomposition of $R_{\alpha,\beta}^{7,2}$ generates an accurate approximation of the exact solution. Furthermore, it follows from and Table 5 and Figure 13 that these approximations are effective in terms of runtime.



Figure 12: Plots of the exact solution of Bagley-Torvik problem (49) vs the approximations via $R_{\alpha,\beta}^{7,2}$ and ml_matrix Matlab function. Short-time and long-time profiles are shown in the left and right figures, respectively.

| | AE | RE | Runtime |
|----------------------|------|----------|---------|
| $R^{7,2}_{lpha,eta}$ | 1.01 | 3.40e-03 | 0.32 |
| matrix ml | 0.05 | 4.83e-05 | 31.16 |

Table 5: The maximum absolute error (AE), maximum relative error (RE), and runtime for computing the solution of Bagley-Torvik problem (49) over the interval [0, 50] with mesh grid size of 0.01.



Figure 13: The runtime in seconds for computing the solution of Bagley-Torvik and Basset problems over the interval [0, 50] with mesh grid size $\Delta t = 0.01, 0.05, 0.1, 0.5$.

8.2.2. The Basset problem

The Basset problem considered in [18]

$$\left[D + \delta^{1-\alpha} C D^{\alpha} + 1\right] u(t) = 1, \qquad u(0) = 0, \quad \delta > 0, \quad \alpha \in (0, 1).$$
(57)

This problem models the dynamics of a sphere immersed in an incompressible viscous fluid subjected to gravity under a hydraulic force. When α is a rational number, $\alpha = p/q$, the exact solution to this problem is

$$u(t) = 1 - \sum_{k=1}^{q} c_k E_{\frac{1}{q}}(a_k t^{\frac{1}{q}}),$$
(58)

where $\{a_k\}$ are the zeros of the polynomial $x^q + \delta^{(1-\frac{p}{q})}x^p + 1$, $c_k = -A_k/a_k$, and $A_k = 1/\prod_{j=1}^q (a_k - a_j), \ j \neq k$.

When $\alpha = 1/2$, problem (57) can be converted into the system

$$^{2}D^{\frac{1}{2}}U(t) = AU(t) + e_{2}, \quad U(0) = U^{0},$$
(59)

where

$$U(t) = (u, {}^{c}D^{\frac{1}{2}}u)^{T}, \qquad U^{0} = (0, 0)^{T}, \qquad e_{2} = (0, 1)^{T},$$

and

$$A = \begin{bmatrix} 0 & 1\\ -1 & -\delta^{1/2} \end{bmatrix}.$$

The exact solution of this system (see [21]) is

$$U(t) = t^{\frac{1}{2}} E_{\frac{1}{2},\frac{3}{2}}(At^{\frac{1}{2}}) e_2, \tag{60}$$

which could be approximated by the partial fraction decomposition of $R_{\alpha,\beta}^{7,2}$.

A comparison between the exact solution (58) and the approximation of (60) for $\delta = 3/7$ is presented in Figure 14. With a maximum relative error of 3.17e-04, over the time interval [0,50] for $\Delta t = 0.01$, the runtime of the $R_{\alpha,\beta}^{7,2}$ approximation is 0.20 seconds whereas the runtime of the matlab function ml_matrix is 10.04 seconds. A detailed comparison of the runtime is included in Figure 13.

9. Concluding remarks

- A unified framework for constructing global Padé approximants of the twoparametric MLF, $E_{\alpha,\beta}(-x)$, x > 0, is presented. In particular, fourth-order global Padé approximants are constructed and tested.
- The numerical experiments indicate that these approximants provide efficient and accurate formulas for computing MLFs. Furthermore, these approximants perform well when used to approximate the MLF of a matrix.
- An algorithm for approximating the inverse function based on the inversion of fourth-order approximants is provided.
- The developed rational approximants will play a pivotal role in developing efficient high-order generalized ETD schemes analogue to the ETD schemes in [6]. This will be explored in a future work.



Figure 14: Plots of the exact solution of Basset problem (58) vs the approximations via $R^{7,2}_{\alpha,\beta}$ and ml_matrix Matlab function. Short-time and long-time profiles are shown in the left and right figures, respectively.

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