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NUMERICAL EXPERIMENTS ON ANALYTICITY OF SOLUTIONS TO FRACTIONAL DIFFERENTIAL EQUATIONS

Hiroshi Fujiwara
Graduate School of Informatics, Kyoto University,
Yoshida-honmachi, Sakyo-ku, Kyoto, 606-8501, Japan
(fujiwara@acs.i.kyoto-u.ac.jp)

Nobuyuki Higashimori
Center for the Promotion of Interdisciplinary Education and Research,
Kyoto University,
Yoshida-honmachi, Sakyo-ku, Kyoto, 606-8501, Japan
(nobuyuki@acs.i.kyoto-u.ac.jp)

and

Hitoshi Imai
Faculty of Science and Engineering, Doshisha University,
1-3 Tatara Miyakodani, Kyotanabe, Kyoto, 610-0394, Japan
(himai@mail.doshisha.ac.jp)

Abstract. In the paper, analyticity of solutions of fractional differential equations is investigated numerically. In numerical computation the Chebyshev spectral collocation method is used for discretization to realize arbitrary order approximation. Multiple-precision arithmetic is also used for arbitrary reduction of rounding error. Some one-dimensional fractional differential equations are solved numerically. Numerical results clarify analyticity of solutions.

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1 Introduction

Recently, there has been a tremendous increase in the use of fractional differential models to simulate dynamics in many fields, e.g. physics, chemistry, biology, engineering and so on [1],[4],[6],[7],[17]. In the models fractional order derivatives are used. They have a long history and they have been studied in the field of fractional calculus. A list of prominent mathematicians contributing to fractional calculus is found in [20]. Besides them, Caputo gave a convenient definition for initial value problems of differential equations as follows [5]: For $0 < \alpha$ non-integer,

$$
{}_{\mathrm{C}}D_0^{\alpha}\, u(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-s)^{n-\alpha-1} \frac{d^n\, u(s)}{ds^n}\, ds, \tag{1}
$$

where Γ is the gamma function, $n = \lceil \alpha \rceil$ is the least integer more than or equal to α, and u is assumed to be sufficiently smooth. This definition is used in the paper because it is convenient for our numerical computation.

It is hard to obtain exact solutions of fractional differential equations, or even if an exact solution is available it may be too complicated to be used in practice. Thus the role of numerical computation becomes important. Various numerical methods to fractional differential equations such as the Adams-type predictor-corrector method, linear multi-step methods, are presented in [1] and [7]. Spectral methods have also been applied to fractional differential equations [7],[9],[21]. As for spectral methods it is well known that they are superior in accuracy [3]. If a function u is m-times continuously differentiable, then $\|u - u_N\| = O(N^{-m})$ where u_N is the N-th order approximate function by the spectral methods, and $\|\cdot\|$ is a suitable norm. This property is called spectral accuracy or infinite-order accuracy. Moreover, if a function u is analytic in a strip of the complex plane, then $\|u - u_N\| = O(e^{-\gamma N})$ with some positive number γ. In [21] numerical results for some fractional differential equations show spectral accuracy.

Spectral methods are roughly divided into the Galerkin type and the collocation type [2],[3]. The latter type is called the spectral collocation method, and it is more convenient for nonlinear problems or higher dimensional problems. In the paper the Chebyshev spectral collocation method is adopted. Although in [7] and [21] spectral collocation methods are already used, by using Chebyshev polynomials we can give a concrete expression of coefficients in the linear combination of basis functions. In the paper multiple-precision arithmetic is also used in numerical computation. To investigate mathematical properties of solutions numerically it is necessary to eliminate the influence of rounding error. The combination of spectral methods and multiple-precision arithmetic was presented in [16] to realize the arbitrary reduction of numerical error. Such reduction is indispensable for direct numerical simulations of inverse problems [10],[13],[15]. By using this combination we also investigated numerically mathematical properties of functions or solutions, for instance, regularity or existence of solutions [8],[14],[19]. In the paper, by using the combination we investigate analyticity of solutions of fractional differential equations.

2 The Chebyshev Spectral Collocation Method

We derive a convenient form of fractional derivatives in terms of the Chebyshev spectral method, which plays an essential role in our numerical studies.

First we briefly recall the Chebyshev spectral collocation method [2]. Let $\tilde{U}_N(x)$ be a polynomial function of degree N defined on the interval $[-1, 1]$. The Chebyshev expansion of $\tilde{U}_N(x)$ is

$$\tilde{U}_N(x) = \sum_{k=0}^{N} \bar{a}_k \; T_k(x), \tag{2}$$

where $T_k(x) = \cos(k \arccos x)$ is the Chebyshev polynomial of order k. We also introduce Chebyshev-Gauss-Lobatto collocation points as follows:

$$\bar{x}_j = \cos\frac{j\pi}{N} \qquad (j = 0, 1, 2, \cdots, N). \tag{3}$$

Letting $\tilde{U}_j = \tilde{U}_N(\bar{x}_j)$, from (2) we have

$$\tilde{U}_j = \sum_{k=0}^{N} \bar{a}_k \; T_k(\bar{x}_j).$$

The coefficients $\bar{a}_k$ are given by the following inverse formula

$$\bar{a}_k = \frac{2}{N\bar{c}_k} \sum_{j=0}^{N} \frac{1}{\bar{c}_j} T_k(\bar{x}_j)\tilde{U}_j, \qquad (k = 0, 1, 2, \ldots, N) \tag{4}$$

where

$$\bar{c}_j = \begin{cases} 2, & j = 0, N, \\ 1, & \text{otherwise.} \end{cases}$$

Substituting (4) to $\bar{a}_k$ in (2) we obtain

$$\tilde{U}_N(x) = \sum_{j=0}^{N} \left(\frac{1}{\bar{c}_j} \sum_{k=0}^{N} \frac{2}{N\bar{c}_k} T_k(\bar{x}_j) T_k(x) \right) \tilde{U}_j.$$

This representation motivates an N-th order approximation $U_N(x)$ to a function $U(x)$ on $[-1, 1]$ as

$$U_N(x) = \sum_{j=0}^{N} \left(\frac{1}{\bar{c}_j} \sum_{k=0}^{N} \frac{2}{N\bar{c}_k} T_k(\bar{x}_j) T_k(x) \right) U_j, \tag{5}$$

where $U_j = U(\bar{x}_j)$. We should remark that if $U(x)$ is a polynomial of degree $m(\leq N)$ then $U(x) = U_N(x)$. The truncation number N in (5) denotes the approximation order. On the other hand, N in (3) denotes the number of collocation points; to be exact, the number is $(N + 1)$. This means that in spectral collocation methods the approximation order can be easily controlled by the number of collocation points. As stated in Introduction, spectral collocation methods are applicable to nonlinear problems or higher dimensional problems. These features are quite convenient to investigate mathematical properties of solutions to various problems.

In spectral collocation methods, differential equations are satisfied at the collocation points. Thus they require the derivative of the approximate function at each collocation point. For instance, the first order derivative of $U_N(x)$ at the collocation point $\overline{x}_i$ is given by differentiating (5):

$$\frac{d}{dx}U_N(\bar{x}_i) = \sum_{j=0}^{N}(D_x)_{i,j}\,U_j = \sum_{j=0}^{N}\left(\frac{1}{\bar{c}_j}\sum_{k=0}^{N}\frac{2}{N\bar{c}_k}T_k(\bar{x}_j)\frac{d}{dx}T_k(\bar{x}_i)\right)U_j, \tag{6}$$

where D_x is called the first order derivative matrix.

Let $u(t)$ be a function defined on $[0,T]$. By substituting $t = \dfrac{T}{2}(x+1)$, $u\left(\dfrac{T}{2}(x+1)\right)$ is a function on $[-1,1]$ and is approximated by the Chebyshev expansion

$$U_N(x) = \begin{pmatrix} T_0(x) & \cdots & T_N(x) \end{pmatrix} \begin{pmatrix} \overline{a}_0 \\ \vdots \\ \overline{a}_N \end{pmatrix}.$$

By using a square matrix $\tilde{T} = \left(\tilde{T}_{kj}\right)$ of order $N+1$ with entries $\tilde{T}_{kj} = \dfrac{2}{N\overline{c}_k\overline{c}_j}T_k(\overline{x}_j)$, the inverse formula (4) in the matrix form is

$$\begin{pmatrix} \overline{a}_0 \\ \vdots \\ \overline{a}_N \end{pmatrix} = \tilde{T}\begin{pmatrix} U_0 \\ \vdots \\ U_N \end{pmatrix},$$

where $U_j = u\left(\dfrac{T}{2}(\overline{x}_j+1)\right)$. Let C be a square matrix of order $N+1$ which satisfies

$$C\begin{pmatrix} 1 \\ \frac{T}{2}(x+1) \\ \vdots \\ \left(\frac{T}{2}\right)^N (x+1)^N \end{pmatrix} = \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_N(x) \end{pmatrix}. \tag{7}$$

We remark that $\tilde{T}$ and C are constant matrices. They lead to the expression

$$U_N(x) = \begin{pmatrix} 1 & \frac{T}{2}(x+1) & \cdots & \left(\frac{T}{2}(x+1)\right)^N \end{pmatrix} C^T\tilde{T}\begin{pmatrix} U_0 \\ \vdots \\ U_N \end{pmatrix},$$

where C^T is the transpose of C. Let $t_j = \dfrac{T}{2}(\overline{x}_j+1)$, $u_j = u(t_j)$, and $u_N(t) = U_N(x)$ with $t = \dfrac{T}{2}(x+1)$. Then $u_j = U_j$ and the function u_N is an approximation to u and is written as

$$u_N(t) = \begin{pmatrix} 1 & t & \cdots & t^N \end{pmatrix} C^T \tilde{T} \begin{pmatrix} u_0 \\ \vdots \\ u_N \end{pmatrix}.$$

This immediately leads to the fractional derivative of u_N at t_i as

$${}_{\mathrm{c}}D_0^{\alpha} u_N(t_i) = \begin{pmatrix} {}_{\mathrm{c}}D_0^{\alpha}[1](t_i) & {}_{\mathrm{c}}D_0^{\alpha}[t](t_i) & \cdots & {}_{\mathrm{c}}D_0^{\alpha}[t^N](t_i) \end{pmatrix} C^T \tilde{T} \begin{pmatrix} u_0 \\ \vdots \\ u_N \end{pmatrix},$$

which is a linear combination of u_j, $j = 0, \ldots, N$, and is similar to (6). It should be emphasized that the Caputo derivatives of the unknown function at each collocation points ${}_{\mathrm{c}}D_0^{\alpha}[t^k](t_i)$ are easily calculated since the Caputo derivatives of monomials t^k for a nonnegative integer k are given by

$${}_{\mathrm{c}}D_0^{\alpha}[t^k] = \begin{cases} 0, & 0 \le k < \alpha, \\ \frac{\Gamma(k+1)}{\Gamma(k+1-\alpha)} t^{k-\alpha}, & \alpha \le k. \end{cases}$$

It is noted in [21] that the entries of C are calculated by the use of inverse of the Vandermonde matrix which is obtained by substituting $N+1$ collocation points $\overline{x}_j$, $j = 0, 1, \ldots, N$, into (7). However, the entries of C are calculated explicitly as follows. For the purpose, we introduce two square matrices $F = \begin{pmatrix} f_{kj} \end{pmatrix}$ and $L = \begin{pmatrix} \ell_{kj} \end{pmatrix}$ of order $N+1$, which satisfy

$$\begin{pmatrix} T_0(x) \\ \vdots \\ T_N(x) \end{pmatrix} = F \begin{pmatrix} 1 \\ x \\ \vdots \\ x^N \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 \\ x \\ \vdots \\ x^N \end{pmatrix} = L \begin{pmatrix} 1 \\ \frac{T}{2}(x+1) \\ \vdots \\ \left(\frac{T}{2}\right)^N (x+1)^N \end{pmatrix}.$$

Firstly, the entries f_{kj} are calculated from the recurrence relation $T_0(x) = 1$, $T_1(x) = x$ and $T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x)$. Secondly, it follows from the binomial expansion that

$$x^k = (x+1-1)^k = \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} (x+1)^j.$$

Since $(x+1)^j$, $j = 0, \ldots, N$, are linearly independent, ℓ_{kj} is given by

$$\ell_{kj} = \begin{cases} (-1)^{k-j} \left(\dfrac{2}{T}\right)^j \dbinom{k}{j}, & j \le k, \\ 0, & k < j. \end{cases}$$

Finally the product of two lower triangular matrices gives $C = FL$.

3 Numerical Evaluation of Fractional Derivatives

This section is devoted to investigate accuracy of numerical integration appearing in (1) and computational environments.

The integrand in (1) has a singularity at boundary $s = t$, and thus special attentions should be paid for the sake of reliable and accurate computation. The use of double exponential rule [18] is known as a novel method to overcome the difficulty. It is also convenient due to returning numerical results in given tolerance automatically.

We demonstrate an example with $0 < \alpha < 1$ and $u(t) = t^2$. Using the standard double exponential transformation $\phi(y) = \tanh\left(\frac{\pi}{2}\sinh y\right)$, the evaluation of integral at $t = 1$ is

$$ {}_{\mathrm{c}}D_0^{\alpha} u(1) = \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^{\infty} \frac{\phi(y)+1}{\left(\frac{1-\phi(y)}{2}\right)^{\alpha}} \frac{\phi'(y)}{2}\, dy $$

by introducing the discretization parameter $h > 0$ and $y_k = kh$, $k \in \mathbb{Z}$, "the composite trapezoidal rule" gives an approximate series as

$$ \approx \frac{1}{\Gamma(1-\alpha)} \sum_{k\in\mathbb{Z}} \frac{\phi(y_k)+1}{\left(\frac{1-\phi(y_k)}{2}\right)^{\alpha}} \frac{\phi'(y_k)}{2} h $$

which is truncated to a finite sum as

$$ \approx \frac{1}{\Gamma(1-\alpha)} \sum_{K_0\le k\le K_1} \frac{\phi(y_k)+1}{\left(\frac{1-\phi(y_k)}{2}\right)^{\alpha}} \frac{\phi'(y_k)}{2} h $$

with some integers K_0 and K_1.

As $|k| \to \infty$, $\phi'(y_k)$ converges to the zero more rapidly than growth of the integrand caused by the singularity, and their products and accumulations are negligible for sufficiently large $|k|$. Therefore choice of h, K_0, and K_1 is crucial for accuracy of numerical integration. Table 1 and Table 2 show numerical evaluation of

$$ I_h = \frac{1}{\Gamma(1-\alpha)} \sum_{K_0\le k\le K_1} \frac{\phi(y_k)+1}{\left(\frac{1-\phi(y_k)}{2}\right)^{\alpha}} \frac{\phi'(y_k)}{2} h $$

with $\alpha = 0.5,\ 0.9$ respectively. In the tables, we show discretization and truncation parameters as $L = K_0 h$, $U = K_1 h$, and $K = K_1 - K_0$. Values of the exact solution

$$ {}_{\mathrm{c}}D_0^{\alpha}\left[t^2\right]\Big|_{t=1} = \frac{2}{\Gamma(3-\alpha)} $$

are also shown in tables.

From Table 1, both double precision arithmetic and 100 decimal digit computation enable us to find approximate values with $(L, U) = (-5, 3.16)$ for $\alpha = 0.5$. On the other hand, for $\alpha = 0.9$, parameters $(L, U) = (-5, 5)$ and $K \geq 16$ in 100 decimal digit return approximations while the double precision arithmetic returns infinity if U is greater

Table 1: Numerical integration I_h with $\alpha = 0.5$.

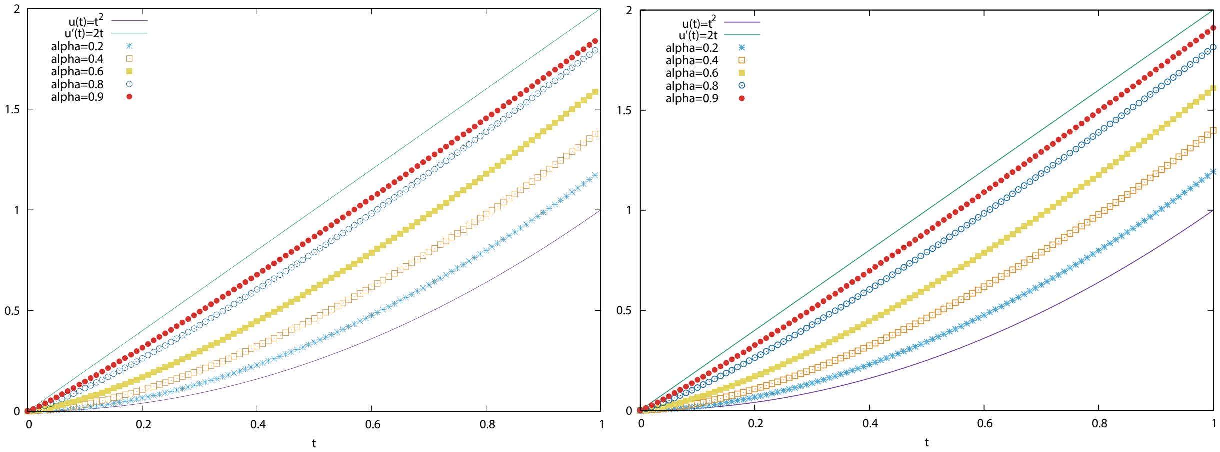
L	U	K	double precision	100 digits
-5.00	3.16	8	1.50652114572	1.50652118788
		16	1.50451382597	1.50451384705
		32	1.50450554499	1.50450555553
-5.00	3.17	8	$+\infty$	1.50798169193
		16	$+\infty$	1.50451519723
		32	$+\infty$	1.50450555566
exact value			1.50450555613...	

Table 2: Numerical integration I_h with $\alpha = 0.9$.

L	U	K	double precision	100 digits
-5.00	3.16	8	1.87072828925	1.90636895125
		16	1.87900443987	1.89682476417
		32	1.87188368373	1.88079405669
-5.00	3.17	8	$+\infty$	1.90645242453
		16	$+\infty$	1.89759689138
		32	$+\infty$	1.88210055004
-5.00	5.00	8	$+\infty$	1.90117136452
		16	$+\infty$	1.91113179851
		32	$+\infty$	1.91115819291
exact value			1.91115819293...	

than or equal to 3.17. This means that double precision arithmetic is not enough for numerical evaluation of fractional derivatives without special treatments of singularities in I_h, especially when the power $-\alpha$ is close to -1. In our numerical computation, *exflib* [11] is used for multiple-precision arithmetic.

Figure 1 shows profiles of fractional derivatives ${}_{\mathrm{c}}D_0^{\alpha}u(t)$ for $u(t) = t^2$ obtained by numerically integrating (1). Figure 1(a) and (b) are processed with double precision arithmetic and 100 decimal digits arithmetic respectively. We set $(L, U) = (-5, 3.16)$ in double precision arithmetic, and $(L, U) = (-5, 5)$ in 100 decimal digits arithmetic, with sufficiently large K. Obviously, results for $\alpha = 0.9$ do not coincide. This also shows that double precision is not enough for reliable computations. More detail discussions and other numerical examples will be found in [12].



(a) Results by double precision (b) Results by 100 decimal digits

Figure 1: Fractional derivatives ${}_{\mathrm{c}}D_0^{\alpha}u(t)$ of $u(t) = t^2$.

4 Numerical Results for Fractional Differential Equations

In this section we shall demonstrate some examples which shows efficiency of combination of the Chebyshev spectral method and multiple-precision arithmetic to achieve arbitrary accurate numerical solutions to fractional order differential equations.

Example 1.

$$\begin{aligned} &u^{(1/3)}(t) = f(t), \quad 0 < t < 3, \\ &u(0) = 0. \end{aligned}$$

Three cases are considered: $f(t) = \frac{5\,!}{\Gamma(17/3)}t^{14/3}$, $\frac{10\,!}{\Gamma(32/3)}t^{29/3}$, and $\frac{15\,!}{\Gamma(47/3)}t^{44/3}$. The exact solutions are $u(t) = t^5$, t^{10}, and t^{15} respectively. Since each solution is a monomial, it is exactly treated by the Chebyshev spectral method, and hence only rounding errors appear as numerical errors.

In Figure 2, the horizontal axis is the spectral degree N and the vertical axis shows errors in numerical results:

$$\max_{0 \le j \le N} |u(\overline{x}_j) - u_N(\overline{x}_j)|$$

in the logarithmic scale. In the figure, purple, green, and blue graph represent numerical errors for $u(t) = t^5$, t^{10}, and t^{15} respectively. In each color, plus (+) sign and cross ($\times$) are error in 50 decimal digits and 100 decimal digits respectively. In each setting, behaviour of errors suddenly changes at a certain order N_0. More precisely, when N becomes larger than or equal to N_0, the numerical errors are less than 10^{-50} or 10^{-100} which correspond to the rounding errors in each computation. This indicates that the solution is a polynomial of degree almost N_0.

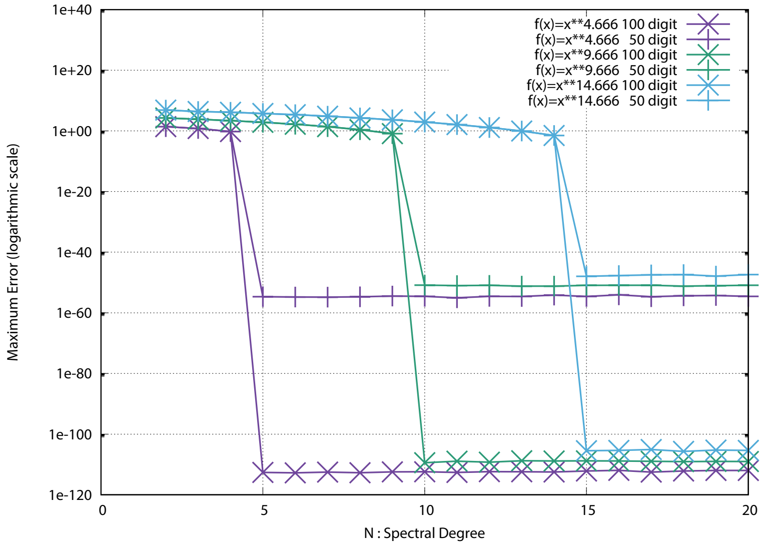
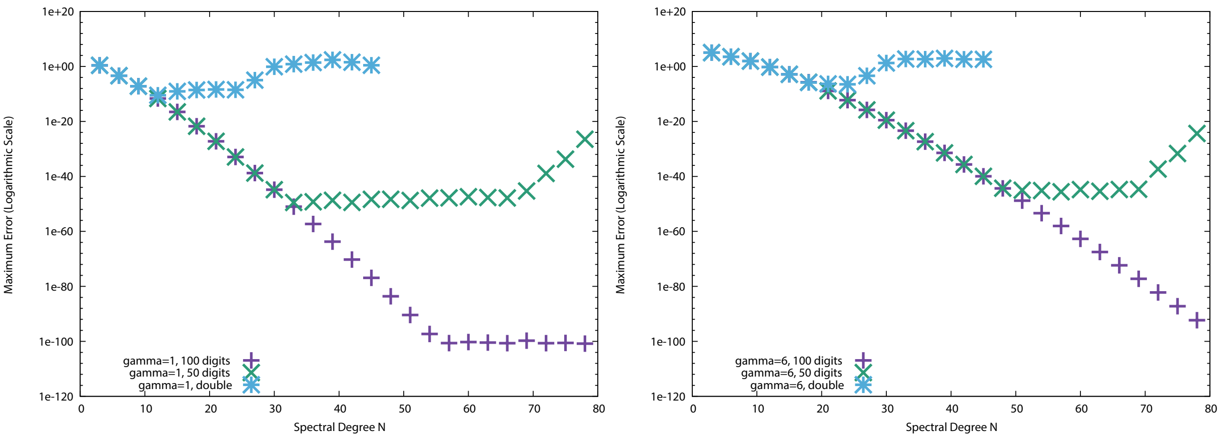


Figure 2: Error decay for Example 1, the exact solutions are monomials.

Example 2. [9]

$$
\begin{aligned}
&u^{(5/2)}(t) - 3u^{(2/3)}(t) = f(t), \qquad 0 < t \leq 1, \\
&u(0) = 1, \quad u'(0) = \beta, \quad u''(0) = \beta^2.
\end{aligned}
$$

We set the exact solution $u(t) = e^{\beta t}$, and calculate $f(t)$ as the left-hand side of the equation by using (1). Figure 3 shows numerical results by double precision (blue), 50 decimal digits (green), and 100 decimal digits (purple). The error decreases exponentially until the level of rounding error is almost reached. This behavior of errors is expected from the property of the spectral methods.



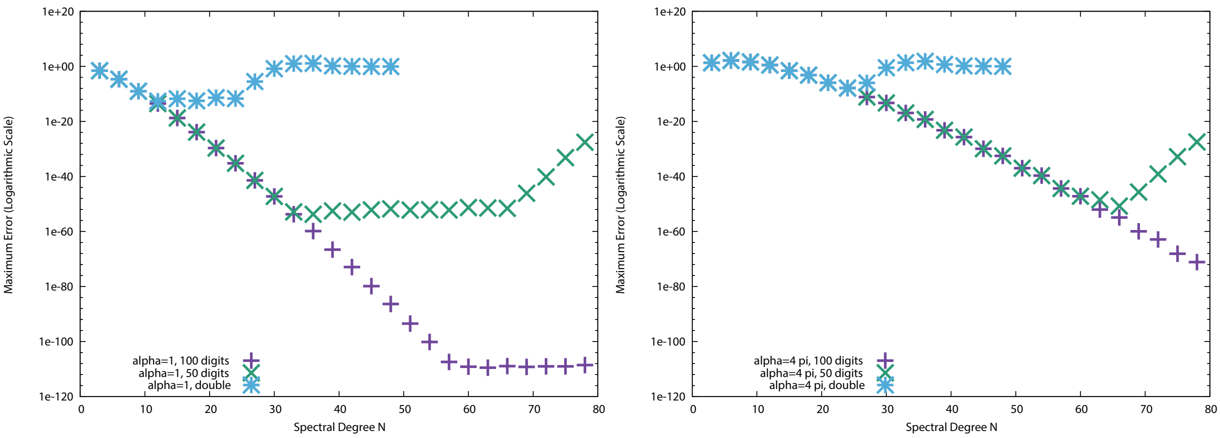
(a) $\beta = 1$ (b) $\beta = 6$

Figure 3: Error decay for Example 2, the exact solution is $e^{\beta t}$.

Example 3. [9]

$$
\begin{aligned}
&u''(t) + u^{(1.5)}(t) + u(t) = f(t), \qquad 0 < t \leq 1,\\
&u(0) = 0, \quad u'(0) = \omega.
\end{aligned}
$$

The equation is known as the Bagley-Torvik equation. We set the exact solution $u(t) = \sin \omega t$. Then $f(t)$ is calculated by using (1). Numerical results in several precisions are shown in Figure 4. The error decreases similarly in the preceding example, since the exact solution is also analytic in this example.



(a) $\omega = 1$ (b) $\omega = 4\pi$

Figure 4: Error decay for Example 3, the exact solution is $\sin \omega t$.

Example 4. In the same equation and initial condition as Example 1, we adopt $f(t) = \Gamma(7/3)t$, and the exact solution is $u(t) = t^{4/3}$. Figure 5 shows numerical results, where both the horizontal and vertical axes are in the logarithmic scale. In this setting numerical errors decay as $O(N^{-2.66})$, which is not exponential decay but polynomial decay with respect to N. This suggests that the exact solution is not analytic.

5 Conclusion

In the paper, by using the Chebyshev spectral collocation method a concrete expression of coefficients in the linear combination of basis functions is derived. It is used for solving one-dimensional fractional differential equations numerically. We also investigate analyticity of solutions numerically. To do so, in numerical computation the multiple-precision arithmetic is used to estimate the influence of rounding error. Numerical results are very satisfactory. Spectral accuracy is seen and it shows analyticity of solutions. Moreover, when exact solutions are monomials, numerical results are succeeded to determine the degree of monomials.

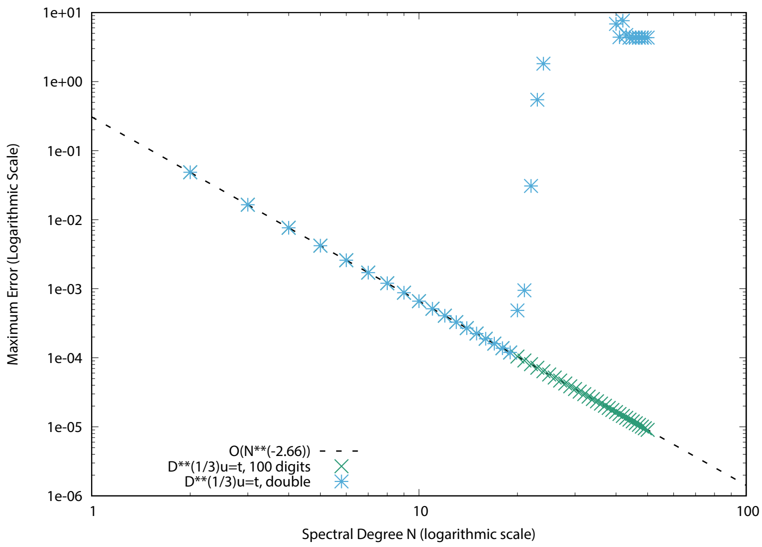


Figure 5: Error decay for Example 4 in double precision arithmetic (Blue) and 100 decimal digits (Green), the exact solution is $t^{4/3}$.

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