Numerical Treatment of Differential Equations of Fractional Order

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Abstract: The collocation approximation with polynomial splines is applied to differential equations of fractional order and the systems of equations characterizing the numerical solution are determined. In particular, the weight matrices resulting from the fractional derivative of the spline are deduced and decomposed for numerical implementation. The main result of this paper is the simplification of the numerical method under a specific smoothness condition on the chosen splines. Numerical results conclude the work and show that the expected qualitative behaviour is given by collocation approximation. Moreover, a method of decomposition is suggested for multiple–term fractional differential equations.

1 Introduction

The question 'what could be a derivative of non integer order' arose in the year 1695, when L'Hôpital asked Leibniz for an interpretation of $D^\alpha f$ where α is a fraction. The theory for derivatives of fractional order was developed in the 19th century. Two different approaches exist. They are equivalent for a wide class of functions (for more details we refer to Miller and Ross [1993]).

The Grünwald–Letnikov definition generalizes the expression of the N-th derivative as a limit of backward difference quotients and gives for positive α

$$D^\alpha y(t) = lim_{n\to\infty} \left(\frac{t}{n}\right)^{-\alpha} \sum_{j=0}^{n} (-1)^j \binom{\alpha}{j} y\left(t - j\frac{t}{n}\right) \quad .$$

On the other hand the Riemann–Liouville definition has as a starting point Cauchy's integral formula which leads to the definition of D^α for $N < \alpha \leq N+1$, $N \in \mathbb{N}$

$$D^\alpha y(t) = D^{N+1} \frac{1}{\Gamma(N+1-\alpha)} \int_0^t (t-s)^{N-\alpha}\, y(s)\, ds \quad .$$

Consequently D^α is the left inverse operator of the Abel–integral operator

$$J^\alpha y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1}\, y(s)\, ds \quad ,$$

(i.e. $D^\alpha J^\alpha = Id$) and $D^\alpha y(t) = D^{N+1} J^{N+1-\alpha} y(t)$. This work is based on the latter definition.

In contrast to derivatives of integer order, which depend only on the local behaviour of the function, derivatives of fractional order involve the whole history of the function in a weighted form. This memory effect leads to many applications of differential equations of fractional order. For example, phenomena in electromagnetics, acoustics, viscoelasticity, electrochemistry and materials science are described by differential equations of fractional order (see for example Beyer and Kempfle [1993]; Ochman and Makarov [1993]; Michalski [1993]; Glöckle and Nonnenmacher [1991]; Babenko [1994a, 1994b]; Mainardi [1994]; Gaul, Klein and Kempfle [1991]; Mann and Wolf [1951]). Fractional calculus also has applications in probability theory, classical analysis and for solving partial differential equations of integer order (see Oldham and Spanier [1974]).

2 Results for basic linear differential equations of fractional order

To give an insight into differential equations of fractional order let us generalize the relaxation equation

$$Dy(t) = -\lambda \cdot y(t) \qquad \text{with} \qquad y(0) = y_0$$

with the solution $y(t) = y_0 \cdot exp(-\lambda t)$ and the oscillation equation

$$D^2 y(t) = -\lambda^2 \cdot y(t) \qquad \text{with} \qquad y(0) = y_0 \quad \text{and} \quad y'(0) = y'_0$$

with the solution $y(t) = y_0 \cdot cos(\lambda t) + y'_0 \frac{1}{\lambda} sin(\lambda t)$.

In view of the applications in science, where the values of fractional derivatives at the initial point 0 are most unlikely to be known but where derivatives $y^{(s)}(0)$ of integer order s are given, we incorporate the initial data. For arbitrary positive α with $N < \alpha \leq N+1$ we obtain the equation

$$D^\alpha \left(y(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0) \right) = -\lambda^\alpha \cdot y(t) \tag{1}$$

with given initial data $y^{(s)}(0)$ $(s = 0, \cdots, N)$. Notice that for integer values α we have $D^\alpha \left(y(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0) \right) = D^\alpha \left(y(t) \right)$.

Gorenflo and Rutman [1995] analysed the solution of (1) in more detail for values $\alpha \in (0, 2)$:

Theorem 1 (Gorenflo and Rutman [1995]) *For $0 < \alpha \leq 1$ the unique solution of the equation*

$$D^\alpha \left(y(t) - y_0 \right) = -\lambda^\alpha \cdot y(t) \quad \textit{with } y(0) = y_0 \tag{2}$$

is given by

$$y(t) = y_0 w_0(t) \quad \textit{with } w_0(t) = E_\alpha\left(-(\lambda t)^\alpha\right) \quad .$$

Furthermore, $w_0(t) = 1 - \frac{(\lambda t)^\alpha}{\Gamma(1+\alpha)} + O\left((\lambda t)^{2\alpha}\right)$ *as* $t \to 0$ *while* $w_0(t) \approx \frac{1}{\Gamma(1-\alpha)}(\lambda t)^{-\alpha}$ *as* $t \to \infty$.

Here $E_\alpha(z)$ denotes the Mittag–Leffler function

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}$$

(for more details see Erdelyi etc. [1955]), which generalizes the exponential function.

We could say (2) 'extrapolates' the relaxation equation to so called 'ultraslow' processes. This means the smaller the value of $\alpha < 1$, the faster the rate of decrease of the solution for small t and the slower the rate of decrease in the solution as $t \to \infty$ (see also numerical results later on).

Theorem 2 (Gorenflo and Rutman [1995]) *For* $1 < \alpha \leq 2$ *the unique solution of the equation*

$$D^\alpha\left(y(t) - y_0 - t y_0'\right) = -\lambda^\alpha \cdot y(t) \quad \textit{with } y(0) = y_0 \textit{ and } y'(0) = y_0' \tag{3}$$

is given by

$$y(t) = y_0 w_0(t) + y_0' w_1(t) \quad \textit{with } w_1(t) = \int_0^t w_0(s)\, ds \quad .$$

$w_0(t) \approx \frac{1}{\Gamma(1-\alpha)}(\lambda t)^{-\alpha}$ *and* $w_1(t) \approx \frac{1}{\lambda\Gamma(2-\alpha)}(\lambda t)^{1-\alpha}$ *as* $t \to \infty$. *Furthermore,* w_0 *and* w_1 *have a finite number of positive zeros (*w_0 *has an odd number while* w_1 *has an even number of zeros) and* w_0 *tends to 0 from below as* $t \to \infty$.

The equation (3) 'interpolates' between the relaxation equation and the oscillation equation (see numerical results in section 6). Further particulars about the decay and the location of the zeros can be found in Gorenflo and Mainardi [1996].

Mathematicians have concentrated so far on the theoretical analysis of the solutions of differential equations of non integer order (Babenko [1994a, 1994b], Gorenflo and Rutman [1995], Samko, Kilbas and Marichev [1993], Podlubny [1994b] etc.). However, in spite of a large number of recently formulated applications, the state of the art is far less advanced in the numerical treatment.

For fractional derivatives and integrals Lubich [1986a] introduced and analysed fractional multistep methods. In his following papers [1985, 1986b] this method is applied to Abel–integral equations and is thoroughly investigated concerning stability properties and convergence. On the other hand, Brunner applied the collocation method to Abel–integral equations in several modified ways and analysed its convergence (Brunner [1983, 1985], Brunner and van der Houwen [1986]). Stability analysis hereof can be found in Blank [1995, 1996]. Yet, to the author's knowledge the only work on numerical treatment of *differential* equations of fractional order is by Podlubny [1994a, 1995]. He applies the fractional Euler method –a discretization of the Grünwald–Letnikov definition of the derivative– to a number of test problems.

The aim of this paper is to contribute toward narrowing the existing gap of computational treatment of fractional differential equations by discussing the application of the collocation method and by suggesting a method of decomposition.

Of most interest for fractional relaxation and oscillation is the qualitative behaviour (that is the number and location of the zeros, long time behaviour and damped oscillation). The first target is to develop numerical methods which reflect this behaviour rather than enforcing high convergence order.

In view of the fact that the Mittag–Leffler functions are still not analyzed to the extent that they can be pictured, graphical representations of the approximate solutions for differential equations (2) and (3) are particularly desired. Furthermore, we want to remark that there is a great demand for efficient numerical methods for computing Mittag–Leffler functions for large negative arguments.

3 Collocation method with polynomial splines

The essential steps of the following analysis carry over to nonlinear differential equations of fractional order. Hence we focus on the linear equation

$$D^\alpha \left(y(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0) \right) = -\lambda^\alpha \cdot y(t) + f(t) \tag{4}$$

with $N < \alpha \leq N+1$, $N \in \mathbb{N}$, and incorporated given initial data $y^{(s)}(0)$ ($s = 0, \ldots, N$).

To retain the essential feature of differential equations of noninteger order in the numerical approach, we apply the collocation method with polynomial splines. Other than for differential equations of integer order, collocation with nonsmooth, or even with discontinuous splines, is nevertheless appropriate to approximate the solution of (4), since the given initial values are incorporated in the equation.

Assume we have an equidistant mesh $t_n = n \cdot h$. Furthermore, the numerical solution u shall be r–times globally continuously differentiable and a polynomial spline. ($r = -1$ denotes the discontinuous splines). On each subinterval $[t_j, t_{j+1}]$ the spline u can be described by piecewise polynomials

$$u(t_j + vh) = \sum_{l=0}^{m-1} a_l^{(j)} v^l \quad (v \in [0,1]) \quad .$$

Define $k = m - (r+1)$ and choose k collocation parameters $0 < c_1 < \ldots < c_k \leq 1$. Then the collocation solution is uniquely given by the following conditions:

$$D^s u(t)|_{t=0} = y^{(s)}(0) \quad s = 0, \ldots, r \tag{5}$$

and u satisfies the functional equation (4) in the collocation points $t_{n,i} = t_n + c_i h$ for $i = 1, \ldots, k$ and $n \in \mathbb{N}$, i.e.:

$$D^\alpha \left(u(t_{n,i}) - \sum_{s=0}^{N} \frac{1}{s!} t_{n,i}^s y^{(s)}(0) \right) = -\lambda^\alpha \cdot u(t_{n,i}) + f(t_{n,i}) \tag{6}$$

In general this leads to 'singular' weights due to the fact that (for details see section 4):

$$\begin{aligned} D^\alpha u(t)|_{t=t_{n,i}} &\approx D^\alpha (v^s)|_{t=t_{n,i}} \ (s = 0, \ldots, m-1) \\ &\approx (t_j + c_l h)^{s-\alpha} \ (j = 0, \ldots, n; l = 0, \ldots, k) \end{aligned}$$

which have negative exponents for $s \leq N$.

However, as we will see in section 5, by choosing smooth splines (more precisely N–times continuously differentiable splines) with the above given initial conditions we can eliminate the 'singular' weights. This is of great advantage for the numerical evaluation since it avoids rounding errors. Furthermore, the resulting system of equations simplifies considerably.

Remark 1 *While in most cases the Lagrange representation for splines for collocation approximation is chosen, it is more convenient to use the representation $\sum_{l=0}^{m-1} a_l v^l$ in this case, since the description of the resulting weight matrices simplifies and emphasizes the main structure.*

4 Derivation of the resulting weights and equations

To set up an equation, that can be coded efficiently in a computer program, the first step is to calculate

$$D^\alpha \left(\sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0) \right) |_{t=t_{n,i}} \text{ and } D^\alpha \left(u(t) \right) |_{t=t_{n,i}} \quad .$$

We will apply the following well known result for fractional derivatives (see for example Oldham and Spanier [1974]).

Lemma 1 *For $\nu \geq 0$, $\mu > -1$ and $t > 0$*

$$D^\nu t^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\nu+1)} t^{\mu-\nu} \quad .$$

This result yields immediately

Corollary 1 *For $\alpha \geq 0$ we have*

$$D^{\alpha}\left(\sum_{s=0}^{N}\frac{1}{s!}t^{s}y^{(s)}(0)\right)|_{t=t_{n,i}} = \frac{h^{-\alpha}}{\Gamma(1-\alpha)}\sum_{s=0}^{N}y^{(s)}(0)h^{s}\left(\prod_{p=1}^{s}\frac{1}{(p-\alpha)}\right)(n+c_i)^{s-\alpha} \quad .$$

(Here and in the following we will use the notation $\prod_{p=1}^{0} a_p := 1$ for arbitrary a_p.)

The calculation of the fractional derivative of a polynomial spline requires deeper consideration, remembering that not only the local behaviour is involved but the whole history of the spline.

$$\begin{aligned}
D^{\alpha}\left(u(t)\right)|_{t=t_{n,i}} &= \frac{h^{N+1-\alpha}}{\Gamma(N+1-\alpha)}\left[h^{-(N+1)}D_{c_i}^{N+1}\int_0^{c_i}(c_i-s)^{N-\alpha}u_n(s)ds\right. \\
&\quad \left.+\sum_{j=0}^{n-1}h^{-(N+1)}D_{n-j+c_i}^{N+1}\int_0^1(n-j+c_i-s)^{N-\alpha}u_j(s)ds\right] \\
&= \frac{h^{-\alpha}}{\Gamma(N+1-\alpha)}\left[\sum_{l=0}^{m-1}a_l^{(n)}D_{c_i}^{N+1}\int_0^{c_i}(c_i-s)^{N-\alpha}s^l ds\right. \\
&\quad \left.+\sum_{j=0}^{n-1}\sum_{l=0}^{m-1}a_l^{(j)}D_{n-j+c_i}^{N+1}\int_0^1(n-j+c_i-s)^{N-\alpha}s^l ds\right] \qquad (7)
\end{aligned}$$

We give briefly the main steps for the further evaluation. In particular the equation (8) below leads to remarkable simplifications and is a key for the general calculation of the weights.

Lemma 2
1.)

$$\int(r-s)^{N-\alpha}s^l ds = -(r-s)^{N+1-\alpha}\sum_{j=0}^{l}(-1)^j\binom{l}{j}\frac{1}{N+1-\alpha+j}r^j(r-s)^{l-j}$$

2.)

$$\sum_{j=0}^{m}(-1)^j\binom{m}{j}\frac{1}{a+j} = \left(\prod_{l=0}^{m}\frac{1}{a+l}\right)m! \qquad (8)$$

Proof: 1.) can be shown by applying the product rule after substitution by $v = r-s$; 2.) follows by induction.

□

Combining these two statements and by appropriate transformation of sums involving factorial expressions we obtain:

$$\int_0^r(r-s)^{N-\alpha}s^l ds \quad = \quad \frac{l!}{\prod_{j=0}^{l}(N+1-\alpha+j)}r^{N+1-\alpha+l}$$

$$
\begin{aligned}
\int_0^1 (r-s)^{N-\alpha} s^l ds &= \frac{l!}{\prod_{j=0}^l (N+1-\alpha+j)} \left[r^{N+1-\alpha+l} \right. \\
&\left. -(r-1)^{N+1-\alpha} \sum_{m=0}^{l} \frac{1}{(l-m)!} (r-1)^m \prod_{j=m+1}^{l} (N+1-\alpha+j) \right]
\end{aligned}
$$

This leads to

$$
\begin{aligned}
D_r^{N+1} \int_0^r (r-s)^{N-\alpha} s^l ds &= l! \frac{\Gamma(N+1-\alpha)}{\Gamma(l+1-\alpha)} r^{-\alpha+l} \\
D_r^{N+1} \int_0^1 (r-s)^{N-\alpha} s^l ds &= l! \frac{\Gamma(N+1-\alpha)}{\Gamma(l+1-\alpha)} \left[r^{-\alpha+l} \right. \\
&\left. -(r-1)^{-\alpha} \sum_{m=0}^{l} (r-1)^m \frac{1}{(l-m)!} \prod_{p=m}^{l-1} (1-\alpha+p) \right]
\end{aligned}
$$

(Note: in the case of $\alpha = N+1 \in \mathbb{N}$ the above formulas stay valid).
Therefore we can state

$$
\begin{aligned}
\frac{h^{-\alpha}}{\Gamma(N+1-\alpha)} D_{c_i}^{N+1} \int_0^{c_i} (c_i - s)^{N-\alpha} s^l ds = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} w_{i,l}^{(0)} \\
\frac{h^{-\alpha}}{\Gamma(N+1-\alpha)} D_{n-j+c_i}^{N+1} \int_0^1 (n-j+c_i-s)^{N-\alpha} s^l ds = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} w_{i,l}^{(n-j)}
\end{aligned}
$$

with the weights

$$
\begin{aligned}
w_{i,0}^{(0)} &= c_i^{-\alpha} \\
w_{i,l}^{(0)} &= c_i^{-\alpha+l} \prod_{p=1}^{l} \frac{p}{p-\alpha} \quad (l \geq 1) \\
&\text{and} \\
w_{i,0}^{(j)} &= (j+c_i)^{-\alpha} - (j+c_i-1)^{-\alpha} \\
w_{i,l}^{(j)} &= (j+c_i)^{-\alpha+l} \prod_{p=1}^{l} \frac{p}{p-\alpha} - \sum_{\nu=0}^{l} (j+c_i-1)^{-\alpha+\nu} \left\{ \prod_{p=1}^{\nu} \frac{l-\nu+p}{p-\alpha} \right\} \quad (l \geq 1)
\end{aligned} \tag{9}
$$

for $j \geq 1$. In summary, we can conclude

Corollary 2 *It holds that*

$$
D^\alpha(u(t_n + c_i h) = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \left[\sum_{j=0}^{n} \sum_{l=0}^{m-1} w_{i,l}^{(n-j)} a_l^{(j)} \right] \tag{10}
$$

and

$$
D^s u(t) = h^{-s} \sum_{l=s}^{m-1} l \cdot \ldots \cdot (l-s+1) \cdot v^{l-s} a_l^{(j)} \tag{11}
$$

with $t = t_j + vh$.

Using Corollary 1 and 2 with the weights defined by (9) we can set up explicitly the equations for the numerical solution. First, we give a convenient way of calculating the weight matrices

$$W^{(j)} = \left(w_{i,l}^{(j)}\right)_{\substack{i=1,\ldots,k\\ l=0,\ldots,m-1}} \quad .$$

We define

$$\begin{aligned}
K^{(j)} &= \left((j+c_i)^{-\alpha+l}\right)_{\substack{i=1,\ldots,k\\ l=0,\ldots,m-1}} \qquad \text{and} \qquad P_{diag} = Id \cdot (P_{l,l})_{l=0,\ldots,m-1} \quad , \\
P &= (P_{\nu,l})_{\substack{\nu=0,\ldots,m-1\\ l=0,\ldots,m-1}} \qquad \text{with} \qquad P_{\nu,l} = \begin{cases} 1 & \text{for } \nu = 0 \\ \prod_{p=1}^{\nu} \frac{l-\nu+p}{p-\alpha} & \text{for } \nu \leq l \\ 0 & \text{for } \nu > l \end{cases}
\end{aligned}$$

This yields the simple equations

$$\begin{aligned}
W^{(0)} &= K^{(0)} P_{diag} \\
W^{(j)} &= K^{(j)} P_{diag} - K^{(j-1)} P \qquad (j \geq 1) \qquad . \qquad (12)
\end{aligned}$$

Furthermore, noticing that the first r coefficients of the numerical solution u are given either by the initial conditions or the conditions of smoothness, we set

$$a^{(j)} = \begin{pmatrix} a_0^{(j)} \\ \vdots \\ a_r^{(j)} \end{pmatrix} \qquad \text{and} \qquad b^{(j)} = \begin{pmatrix} a_{r+1}^{(j)} \\ \vdots \\ a_{m-1}^{(j)} \end{pmatrix} \qquad .$$

With the additional notation

$$\begin{aligned}
f^{(j)} &= (f(t_j + c_i h))_{i=1,\ldots,k} \quad , \\
Diff &= (Diff_{s,l})_{\substack{s=0,\ldots,r\\ l=0,\ldots,m-1}} \qquad \text{with} \qquad Diff_{s,l} = \begin{cases} 1 & \text{for } s = 0 \\ \prod_{p=1}^{s} \frac{l+1-p}{p} & \text{for } s \leq l \\ 0 & \text{for } s > l \end{cases} \\
Y0 &= \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \begin{pmatrix} \ddots & & 0 \\ & h^s \prod_{p=1}^{s} \frac{1}{p-\alpha} & \\ 0 & & \ddots \end{pmatrix}_{s=0,\ldots,N} \cdot \left(\; y^{(s)}(0) \; \right)_{s=0,\ldots,N}
\end{aligned}$$

and

$$\begin{aligned}
INV &= \left[\frac{h^{-\alpha}}{\Gamma(1-\alpha)} W^{(0)}|_{l=r+1,\ldots,m-1} + \lambda^{\alpha} \left(\; c_i^l \; \right)_{\substack{i=1,\ldots,k\\ l=r+1,\ldots,m-1}} \right]^{-1} \qquad \in \mathrm{M(k,k)}, \\
STW &= \frac{h^{-\alpha}}{\Gamma(1-\alpha)} W^{(0)}|_{l=0,\ldots,r} + \lambda^{\alpha} \left(\; c_i^l \; \right)_{\substack{i=1,\ldots,k\\ l=0,\ldots,r}}
\end{aligned}$$

(the expression $M|_{l=p,\ldots q}$ refers to the p-th up to the q-th columns of the matrix M), we obtain:

Theorem 3 *The numerical solution u of (4), given by the collocation approximation as described above, is determined by the following systems of equations: on the first subinterval $[0, t_1)$*

$$\begin{aligned} a^{(0)} &= \begin{pmatrix} \ddots & & 0 \\ & h^s \frac{1}{s!} & \\ 0 & & \ddots \end{pmatrix}_{s=0,\ldots,r} \left(y^{(s)}(0)\right)_{s=0,\ldots,r} \\ b^{(0)} &= INV\left\{-STWa^{(0)} + f^{(0)} + K^{(0)}|_{l=0,\ldots,N} Y0\right\} \end{aligned} \tag{13}$$

while on $[t_n, t_{n+1})$ for $n \geq 1$

$$a^{(n)} = Diff \begin{pmatrix} a^{(n-1)} \\ b^{(n-1)} \end{pmatrix} \tag{14}$$

$$b^{(n)} = INV\left\{-STWa^{(n)} + f^{(n)} + K^{(n)}|_{l=0,\ldots,N} Y0 - \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} W^{(n-j)} \begin{pmatrix} a^{(j)} \\ b^{(j)} \end{pmatrix}\right\}$$

These equations for determining the numerical solution are easy to implement, though we want to bring to the reader's attention that $K^{(j)}$ partly consists of the 'singular' weights, which we mentioned at the end of section 3.

5 N-times continuously differentiable splines

Bearing in mind that the incorporated initial values in (4) lead to a solution y, which is N-times differentiable at 0 (from the right), we can use the Taylor expansion of y at 0 and eliminate the possible singular values at 0 for $D^\alpha\left(y(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0)\right)$.

Now, if we choose N-times continuously differentiable splines (i.e. $r = N$), then we expect the same property on the first interval $[0, h)$. That this effect carries over to $D^\alpha\left(u(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0)\right)$ for $t \geq h$ (that means the initial values $y^{(s)}(0)$ and the 'singular' weights are eliminated), is not as obvious. We will, however, show that for all $n \geq 0$

$$\begin{aligned} &\left[D^\alpha\left(u(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0)\right)|_{t=t_{n,i}}\right]_{i=1,\ldots,k} \\ &\qquad = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \sum_{j=0}^{n} W^{(n-j)} \begin{pmatrix} a^{(j)} \\ b^{(j)} \end{pmatrix} - K^{(n)}|_{l=0,\ldots,N} Y0 \\ &\qquad = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \sum_{j=0}^{n} V^{(n-j)} b^{(j)} \end{aligned} \tag{15}$$

with suitable weight matrices $V^{(j)}$, which will be determined below and which have no terms with negative exponents.

In the following we derive (15) and use the notation $M|^{i=p,\dots,q}$ for the matrix, which consists of the p-th up to the q-th rows of M.
Exploiting the initial conditions in (13) we obtain

$$\frac{h^{-\alpha}}{\Gamma(1-\alpha)} P_{diag}|_{l=0,\dots,N}^{\nu=0,\dots,N} a^{(0)} = Y0 \qquad . \tag{16}$$

This yields for $n = 0$

$$\frac{h^{-\alpha}}{\Gamma(1-\alpha)} \left\{ \left[K^{(0)} P_{diag}|_{l=0,\dots,N} \right] a^{(0)} + \left[K^{(0)} P_{diag}|_{l=N+1,\dots,m-1} \right] b^{(0)} \right\} - K^{(0)}|_{l=0,\dots,N} Y0$$
$$= \frac{h^{-\alpha}}{\Gamma(1-\alpha)} K^{(0)} P_{diag}|_{l=N+1,\dots,m-1} b^{(0)} \quad = \frac{h^{-\alpha}}{\Gamma(1-\alpha)} V^{(0)} b^{(0)}$$

with

$$V^{(0)} = K^{(0)}|_{\nu=N+1,\dots,m-1} P_{diag}|_{l=N+1,\dots,m-1}^{\nu=N+1,\dots,m-1} \qquad .$$

(P_{diag} is a diagonal matrix, hence the first $N+1$ rows of $P_{diag}|_{l=N+1,\dots,m-1}$ are zero.)

In case $n \geq 1$ we have

$$\begin{aligned}
&\sum_{j=0}^{n} W^{(n-j)} \begin{pmatrix} a^{(j)} \\ b^{(j)} \end{pmatrix} - \frac{\Gamma(1-\alpha)}{h^{-\alpha}} K^{(n)}|_{l=0,\dots,N} Y0 \\
&\quad = \sum_{j=0}^{n} W^{(n-j)}|_{l=0,\dots,N} a^{(j)} - K^{(n)}|_{\nu=0,\dots,N} P_{diag}|_{l=0,\dots,N}^{\nu=0,\dots,N} a^{(0)} \\
&\qquad + \sum_{j=0}^{n} W^{(n-j)}|_{l=N+1,\dots,m-1} b^{(j)} \\
&\quad = \sum_{j=0}^{n} \left(K^{(n-j)} P_{diag} \right) |_{l=0,\dots,N} a^{(j)} - \sum_{j=0}^{n-1} \left(K^{(n-j-1)} P \right) |_{l=0,\dots,N} a^{(j)} \\
&\qquad - \left(K^{(n)} P_{diag} \right) |_{l=0,\dots,N} a^{(0)} \\
&\qquad + \sum_{j=0}^{n} \left(K^{(n-j)} P_{diag} \right) |_{l=N+1,\dots,m-1} b^{(j)} - \sum_{j=0}^{n} \left(K^{(n-j-1)} P \right) |_{l=N+1,\dots,m-1} b^{(j)} \\
&\quad = \sum_{j=1}^{n} K^{(n-j)} \left\{ P_{diag}|_{l=0,\dots,N} Diff|_{l=0,\dots,N} - P|_{l=0,\dots,N} \right\} a^{(j-1)} \\
&\qquad + \sum_{j=1}^{n} K^{(n-j)} \left\{ P_{diag}|_{l=0,\dots,N} Diff|_{l=N+1,\dots,m-1} - P|_{l=N+1,\dots,m-1} \right\} b^{(j-1)} \\
&\qquad + \sum_{j=0}^{n} K^{(n-j)}|_{\nu=N+1,\dots,m-1} P_{diag}|_{l=N+1,\dots,m-1}^{\nu=N+1,\dots,m-1} b^{(j)}
\end{aligned}$$

It is easy to see that $P_{diag}|_{l=0,\dots,N} Diff|_{l=0,\dots,N} = P|_{l=0,\dots,N}$ and therefore the expressions with $a^{(j)}$ drop away. However $P_{diag}|_{l=0,\dots,N} Diff|_{l=N+1,\dots,m-1}$ is identical to $P|_{l=N+1,\dots,m-1}$ in the first N rows only and zero otherwise.

Hence

$$K^{(n-j)}\left\{P_{diag}|_{l=0,\ldots,N}Diff|_{l=N+1,\ldots,m-1} - P|_{l=N+1,\ldots,m-1}\right\}$$
$$= K^{(n-j)}|_{\nu=N+1,\ldots,m-1}P|_{l=N+1,\ldots,m-1}^{\nu=N+1,\ldots,m-1} \quad .$$

Defining now

$$\begin{aligned}
\mathbb{K}^{(j)} &= K^{(j)}|_{\nu=N+1,\ldots,m-1} = \left((j+c_i)^{N+l-\alpha}\right)_{\substack{i=1,\ldots,k\\ l=1,\ldots,k}} \\
\mathbb{P} &= (\mathbb{P}_{s,l})_{\substack{s=1,\ldots,k\\ l=1,\ldots,k}} = P|_{l=N+1,\ldots,m-1}^{\nu=N+1,\ldots,m-1} \qquad \text{i.e.} \quad \mathbb{P}_{s,l} = \begin{cases} \frac{(l+N)!}{(l-s)!}\prod_{p=1}^{N+s}\frac{1}{p-\alpha} & \text{for } s \le l \\ 0 & \text{for } s > l \end{cases}
\end{aligned}$$

then

$$\begin{aligned}
V^{(0)} &= \mathbb{K}^{(0)}\mathbb{P}_{diag} \\
V^{(j)} &= \mathbb{K}^{(j)}\mathbb{P}_{diag} - \mathbb{K}^{(j-1)}\mathbb{P} \qquad (j \ge 1)
\end{aligned}$$

and we obtain equation (15), namely

$$\left[D^\alpha\left(u(t) - \sum_{s=0}^{N}\frac{1}{s!}t^s y^{(s)}(0)\right)|_{t=t_{n,i}}\right]_{i=1,\ldots,k} = \frac{h^{-\alpha}}{\Gamma(1-\alpha)}\sum_{j=0}^{n}V^{(n-j)}b^{(j)} \qquad .$$

Consequently, with $Diff$ and INV as defined before, or in a rewritten form

$$\begin{aligned}
Diff &= (Diff_{s,l})_{\substack{s=1,\ldots,k\\ l=1,\ldots,k}} \qquad \text{with} \qquad Diff_{s,l} = \begin{cases} \frac{l!}{s!(l-s)!} & \text{for } s \le l \\ 0 & \text{for } s > l \end{cases} \\
INV &= \left[\frac{h^{-\alpha}}{\Gamma(1-\alpha)}\mathbb{K}^{(0)}\mathbb{P}_{diag} + \lambda^\alpha\left(c_i^{N+l}\right)_{\substack{i=1,\ldots,k\\ l=1,\ldots,k}}\right]^{-1}
\end{aligned}$$

and with

$$C = \left(c_i^{\,l}\right)_{\substack{i=1,\ldots,k\\ l=0,\ldots,N}}$$

the systems of equations (13) and (14) simplify for N-times continuously differentiable splines to (17) and (18) below:

Theorem 4 *The numerical solution u of (4), given by the collocation approximation with N-times continuously differentiable splines as described above, is determined by the following systems of equations:*
on the first subinterval $[0,h]$

$$\begin{aligned}
a^{(0)} &= \begin{pmatrix} \ddots & & 0 \\ & h^s\frac{1}{s!} & \\ 0 & & \ddots \end{pmatrix}_{s=0,\ldots,N} \left(y^{(s)}(0)\right)_{s=0,\ldots,N} \\
b^{(0)} &= INV\left\{-\lambda^\alpha C a^{(0)} + f^{(0)}\right\} \qquad (17)
\end{aligned}$$

and for $n \geq 1$ on $[t_n, t_{n+1}]$

$$\begin{aligned} a^{(n)} &= Diff \begin{pmatrix} a^{(n-1)} \\ b^{(n-1)} \end{pmatrix} \\ b^{(n)} &= INV \left\{ -\lambda^\alpha C a^{(n)} + f^{(n)} - \frac{h^{-\alpha}}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} V^{(n-j)} b^{(j)} \right\} \quad . \end{aligned} \tag{18}$$

Remark 2

1. *Note that $V^{(j)}$, C and also INV have no terms with negative exponents, i.e. all 'singular' weights are eliminated.*

2. *While (13) and (14) need $a^{(j)}$ for $j \leq n-1$ and $y^{(s)}(0)$ for $0 \leq s \leq N$ to calculate $b^{(n)}$, these values are unneccessary in (17) and (18). This fact reduces drastically the number of multiplications involved in each step $n \geq 0$ by about $k^3(N + n(m-k))$, where k is the number of collocation parameters.*

3. *The reason for still considering collocation with arbitrary smooth or nonsmooth splines is the restriction on m for smooth splines. That means, while for discontinuous splines we can choose $m = 1$ (piecewise constant splines), we have to have $m \geq N + 2$ in case of N-times differentiable splines. Therefore, the resulting systems of equations have at least the dimension $N + 1$ for $a^{(n)}$ and 1 for $b^{(n)}$, while the dimension could be zero for $a^{(n)}$ and 1 for $b^{(n)}$ in the case of discontinuous splines.*

6 Numerical Examples

As mentioned at the end of section 2 graphical representations of Mittag–Leffler functions are particularly desired. Hence for shortness we selected as numerical examples in this paper test equations, which have Mittag–Leffler functions as solutions.

The following figures reflect the qualitative behaviour of the solutions of the basic linear differential equations of fractional order, which we considered in section 2. We employed the collocation approximation with polynomial splines, which are N-times continuously differentiable. Furthermore, we chose the three collocation points $c_1 = 0.1$, $c_2 = 0.5$ and $c_3 = 1.0$.

By way of example, figures 1-3 show the numerical solutions u of

$$D^\alpha\left(y(t) - 1\right) = -y(t) \quad \text{with} \quad y(0) = 1$$

where $0 < \alpha < 1$. Hence u approximates the Mittag–Leffler function $E_\alpha(-t^\alpha)$. As desired the graphs show the 'extrapolation' of the relaxation solution e^{-t} to the 'ultraslow' relaxation. As described in theorem 1 for the exact solution, at t close to 0 the collocation solutions descend faster for α closer to 0, while for $t \to \infty$ they show 'slower' relaxation. The fastest relaxation occurs for $\alpha = 1$.

$\alpha = 0.1$

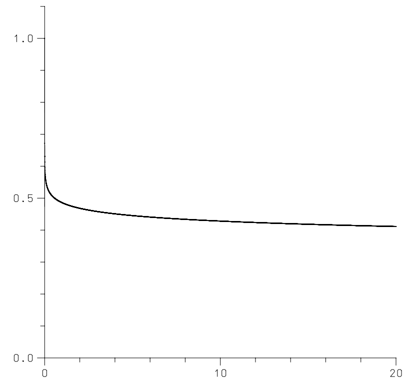

Figure 1

$\alpha = 0.5$

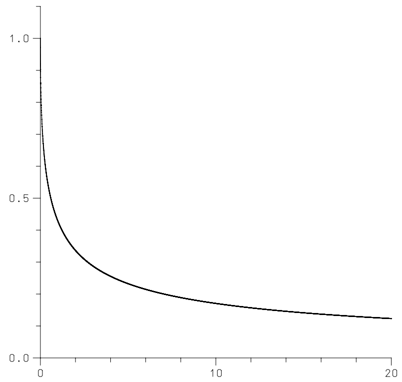

Figure 2

$\alpha = 0.9$

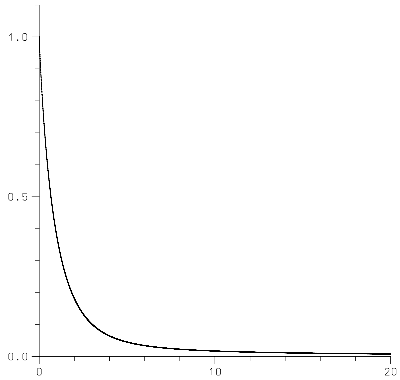

Figure 3

The next figures (4-9) illustrate the 'interpolation' between relaxation and oscillation. The graphs give again the numerical solution to

$$D^{\alpha}\left(y(t) - 1\right) = -y(t) \quad \text{with} \quad y(0) = 1 \text{ and } y'(0) = 0$$

though this time we have $1 < \alpha < 2$. The collocation approximations show the behaviour of the exact solutions (the Mittag–Leffler functions with $\alpha \in (1, 2)$), which means they have an odd number of zeros and tend to 0 as $t \to \infty$ from below. The closer α is to 1 the more they behave like pure relaxation, while the closer α is to 2 the more oscillations occur. The relaxational behaviour is nevertheless preserved.

$\alpha = 1.1$

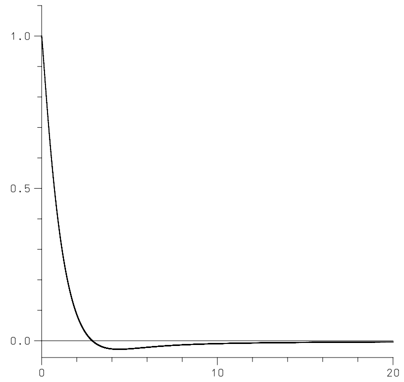

Figure 4

$\alpha = 1.3$

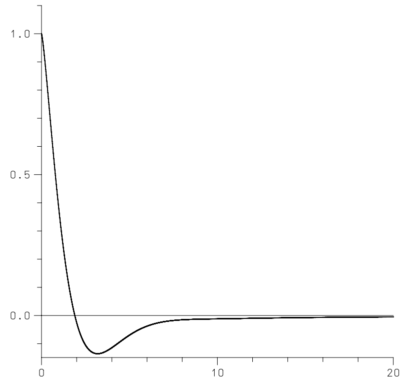

Figure 5

$\alpha = 1.5$

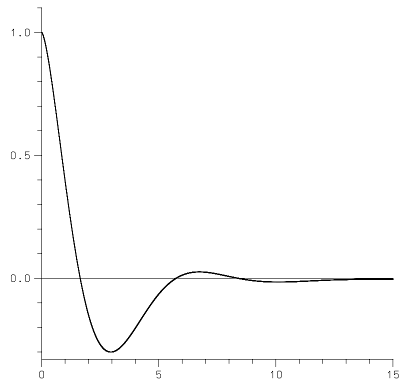

Figure 6

$\alpha = 1.7$

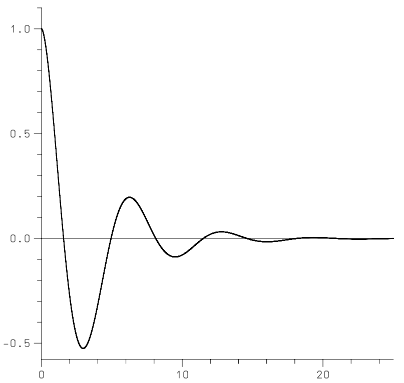

Figure 7

$\alpha = 1.8$

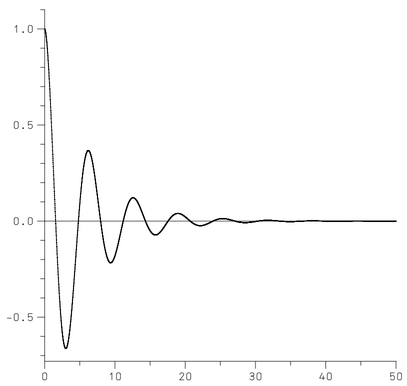

Figure 8

$\alpha = 1.9$

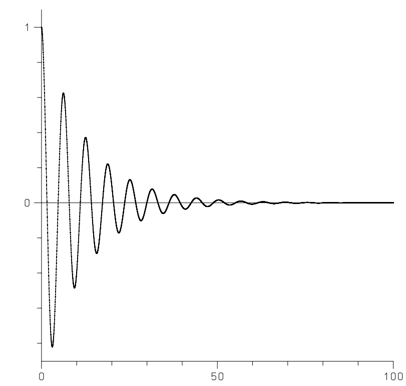

Figure 9

The results of Gorenflo and Mainardi [1996] confirm the validity of the above numerical treatment. This includes in particular the reliability of the location of the zeros.

7 Further work and method of decomposition

In the previous section the numerical solutions of differential equations of fractional order $\alpha \in (0, 2)$ are examined and compared with the analytical results in section 2 for the exact solutions. The following two plots for $\alpha = 2.1$ illustrate the behaviour of solutions for differential equations with $\alpha \in (2, 3)$

$$D^{\alpha}\left(y(t) - y(0) - ty'(0) - \frac{t^2}{2}y^{(2)}(0)\right) = -\lambda^{\alpha} \cdot y(t) \quad . \tag{19}$$

(We chose $y(0) = 1$, $y'(0) = y^{(2)} = 0$ and $\lambda = 1$.)

$\alpha = 2.1$

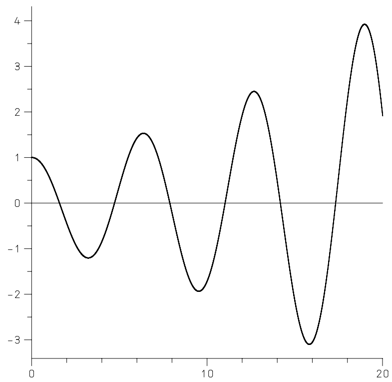

Figure 10

$\alpha = 2.1$

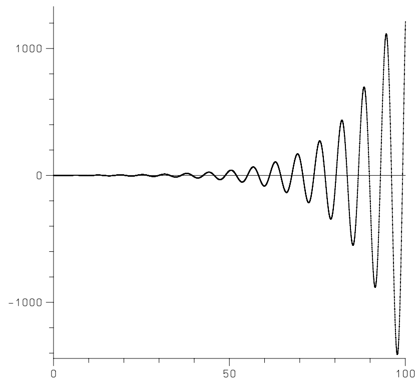

Figure 11

Again, all examples tested suggest that equation (19) interpolates between the oscillation equation ($\alpha = 2$) and the equation with $\alpha = 3$, which has in general an infinite growth. The analytical investigation of the behaviour of the solution of (19), as well as the theoretical analysis of the applied collocation method is subject of further research.

The transference of known numerical methods for differential equations of integer order or integral equations would be the natural approach for the numerical treatment of differential equations of fractional order. A different starting point for the numerical approach is the following decomposition of differential equations of fractional order into a system of differential equations of integer order linked with Abel–Integral equations. We rewrite equation (4) as

$$\begin{aligned} &D^{(N+1)}z(t) = -\lambda^\alpha \cdot y(t) \\ &J^{N+1-\alpha}\left(y(t) - \sum_{s=0}^{N} \frac{1}{s!} t^s y^{(s)}(0)\right) = z(t) \quad . \end{aligned}$$

The open question is, whether the combination of known numerical methods for differential equations of integer order with methods for Abel–Integral equations of the first kind (see Brunner and van der Houwen [1986]) is possible and sensible. We have to take into account that the numerical approach for solving integral equations of the first kind is still a fairly open field.

The great advantage of the method of decomposition would be the use of already existing methods and implemented algorithms and, even more important, the possibility of applying the method of decomposition also to equations, where more than one derivative of fractional order is involved, as for example:

$$D^{\alpha_1}y(t) + D^{\alpha_2}y(t) = f(t, y(t))$$

can be decomposed into the system

$$\begin{aligned} &D^{(N_1+1)}z(t) + D^{(N_2+1)}w(t) = f(t, y(t)) \\ &J^{N_1+1-\alpha_1}y(t) = z(t) \\ &J^{N_2+1-\alpha_2}y(t) = w(t) \quad . \end{aligned}$$

The theory and applications of multiple-term fractional differential equations are commonly known and investigated in the related literature (for example Samko, Kilbas and Marichev [1993]).

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