NUMERICAL APPROXIMATIONS FOR FRACTIONAL DIFFERENTIAL EQUATIONS

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Abstract

The Grünwald and shifted Grünwald formulas for the function $y(x) - y(b)$ are first order approximations for the Caputo fractional derivative of the function $y(x)$ with lower limit at the point $b$. We obtain second and third order approximations for the Grünwald and shifted Grünwald formulas with weighted averages of Caputo derivatives when sufficient number of derivatives of the function $y(x)$ are equal to zero at $b$, using the estimate for the error of the shifted Grünwald formulas. We use the approximations to determine implicit difference approximations for the sub-diffusion equation which have second order accuracy with respect to the space and time variables, and second and third order numerical approximations for ordinary fractional differential equations.

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1 Introduction

Fractional derivatives are an effective tool for modeling diffusion processes in complex systems. Mathematical models with partial fractional differential equations have been used to describe complex processes in physics, biology, chemistry and economics [10-20]. The time fractional diffusion equation is
a parabolic partial fractional differential equation obtained from the heat-diffusion equation by replacing the time derivative with a fractional derivative of order $\alpha$.

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2} + G(x, t).$$

When $0 < \alpha < 1$ the equation is called fractional sub-diffusion equation and it is a model of a slow diffusion process. When the order of the fractional derivative is between one and two the equation is called fractional super-diffusion equation. There is a growing need to design efficient algorithms for numerical solution of partial fractional differential equations. Finite-difference approximations for the heat-diffusion ($\alpha = 2$) and time-fractional diffusion equations have been studied [38-50] for their importance in practical applications as well as for evaluation of their performance.

A common way to approximate the Caputo derivative of order $\alpha$, when $0 < \alpha < 1$, is approximation (6). The finite difference approximation for the fractional sub-diffusion equation which uses approximation (6) for the time fractional derivative and central difference approximation for the second derivative with respect to $x$ has accuracy $O(\tau^{2-\alpha} + h^2)$, where $h$ and $\tau$ are the step sizes of the discretizations with respect to the space and time variables $x$ and $t$.

Tadjeran et al. [23] use the estimate for the error for the Grünwald formula (13) to design an algorithm for a second order numerical approximation of the solution of the space fractional diffusion equation of order $\alpha$, when $1 < \alpha < 2$.

$$\frac{\partial u(x, t)}{\partial t} = d(x) \frac{\partial^\alpha u(x, t)}{\partial x^\alpha} + G(x, t).$$

The algorithm uses a Crank-Nicholson approximation with respect to the time variable $t$ and an extrapolation with respect to the space variable $x$.

Ding and Li [24] compute a numerical solution of the fractional diffusion-wave equation with reaction term

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = K_\alpha \frac{\partial^2 u(x, t)}{\partial x^2} - C_\alpha u(x, t) + G(x, t),$$

where $K_\alpha > 0$ and $C_\alpha > 0$ are the diffusion and reaction coefficients, using a compact difference approximation with an accuracy $O(\tau^2 + h^4)$.

Gorenflo [25] showed that the shifted Grünwald formula $h^{-\alpha} \Delta_{h,\alpha/2}^{\alpha} y(x)$ is a second order approximation for the fractional derivative

$$y^\alpha(x) = h^{-\alpha} \Delta_{h,\alpha/2}^{\alpha} y(x) + O(h^2)$$
when the transition of \(y(x)\) to zero is sufficiently smooth at the lower limit of fractional differentiation. The smoothness condition requires that \(y(b) = 0\). This approximation is a special case of Theorem 1(i), when \(p = \alpha/2\).

There is a significant interest in designing efficient numerical solutions for ordinary and partial fractional differential equations, which stems from the possibility to use fractional derivatives to explain complex processes in nature and social sciences and their relation to integer order differential equations. While approximations of fractional derivatives with accuracy \(O(h^{2-\alpha})\) have been studied extensively, new algorithms with second and higher order accuracy [27-37] have been proposed and successfully applied for numerical solution of ordinary and partial fractional differential equations.

In this paper we construct a second order implicit difference approximation for the fractional sub-diffusion equation (1) and second and third order approximations for the ordinary fractional differential equation

\[
y^{(\alpha)}(x) + y(x) = f(x)
\]

when equations (1) and (2) have sufficiently smooth solutions. In section 3 we use the estimate for the error of the Gr"{u}nwald and shifted Gr"{u}nwald formulas (13) to obtain second and third order approximations for the Gr"{u}nwald and shifted Gr"{u}nwald formulas with weighted averages of Caputo derivatives on a uniform grid, when sufficient number of derivatives of the function \(y(x)\) are equal to zero at the point \(b\). In section 4 we derive recurrence relations (25), (26) and (33) for second and third order approximations to the solution of ordinary fractional differential equation (2) and we determine estimates for the Gr"{u}nwald weights. In section 5 we use approximations (9) and (10) to construct implicit difference approximations (56) and (57) for the solution of the sub-diffusion equation (1) and we show that they have second order accuracy \(O(\tau^2 + h^2)\) with respect to the space and time variables.

2 Preliminaries

The fractional derivatives are generalizations of the integer order derivatives. Let \(y(x)\) be a real-valued function defined for \(x \geq b\). The Riemann-Liouville and Caputo fractional derivatives of order \(\alpha\), when \(0 < \alpha < 1\) are defined as

\[
\begin{align*}
D_{RL}^{\alpha}y(x) &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_{b}^{x} \frac{y(\xi)}{(x-\xi)^{\alpha}} d\xi, \\
D_{C}^{\alpha}y(x) &= y^{(\alpha)}(x) = \frac{d^{\alpha}}{dx^{\alpha}}y(x) = \frac{1}{\Gamma(1-\alpha)} \int_{b}^{x} \frac{y^{(\xi)}(\xi)}{(x-\xi)^{\alpha}} d\xi.
\end{align*}
\]
The Caputo fractional derivative of the constant function 1 is zero and the Riemann-Liouville derivative of 1 is \((x-b)^{-\alpha}/\Gamma(1-\alpha)\). The Caputo derivative of the function \(y(x)\) satisfies

\[
D_x^\alpha y(x) = D_x^\alpha (y(x) - y(b)).
\]

If a function \(y(x)\) is Caputo differentiable of order \(\alpha\) then it is differentiable in the sense of the definition of Riemann-Liouville derivative. The classes Caputo differentiable functions \(C^\alpha\), when \(0 < \alpha < 1\), include the \(C^1\) functions and are suitable for numerical computations for fractional differentiable equations. (For a strict definition of a fractional derivative we assume Lebesgue integration in the definitions of Caputo and Riemann-Liouville fractional derivatives.) The Caputo and Riemann-Liouville fractional derivatives satisfy

\[
D_{RL}^\alpha y(x) = D_x^\alpha y(x) + \frac{y(b)}{\Gamma(1-\alpha)} (x-b)^\alpha.
\]  

The Miller-Ross sequential fractional derivative of order \(\alpha_1 + \alpha_2\) for the Caputo derivative is defined as

\[
y^{(\alpha_1+\alpha_2)}(x) = D_x^{\alpha_1} D_x^{\alpha_2} y(x).
\]

In the special cases \(\alpha_1 = 1\), \(\alpha_1 = 2\) and \(\alpha_2 = \alpha\), when \(0 < \alpha < 1\)

\[
y^{(1+\alpha)}(x) = \frac{d}{dx} y^{(\alpha)}(x), \quad y^{(2+\alpha)}(x) = \frac{d^2}{dx^2} y^{(\alpha)}(x).
\]

The local behavior of a differentiable function is described with its Taylor series and Taylor polynomials. The properties of a function \(y(x)\) close to the lower limit \(b\) can be described with its Caputo and Miller-Ross derivatives at the point \(b\). The following theorem is a generalization of the Mean-Value Theorem for differentiable functions \(57\).

**Theorem.** *(Generalized Mean-Value Theorem)* Let \(y \in C^\alpha[b, x]\). Then

\[
y(x) = y(b) + \frac{(x-b)^\alpha}{\Gamma(\alpha+1)} y^{(\alpha)}(\xi_x) \quad (b \leq \xi_x \leq x).
\]

Fractional Taylor series for Caputo and Miller-Ross derivatives \(57, 58\) can be defined using an approach similar to the derivation of the classical Taylor series which involves only integer order derivatives. While the local
properties of a function at the lower limit $b$ can be explained with its fractional derivatives their values at any other point $x$ depend on the values of the function on the interval $[b, x]$. We can observe a similarity between the Taylor series of the function $y(x)$ and relation (13) for its fractional derivatives and the shifted Grünwald formulas.

Two important special functions in fractional calculus are the gamma and Mittag-Leffler functions. The gamma function has properties

$$\Gamma(0) = 1, \quad \Gamma(z + 1) = z \Gamma(z).$$

When $n$ is a positive integer $\Gamma(n) = (n - 1)!$. The one-parameter and two-parameter Mittag-Leffler functions are defined for $\alpha > 0$ as

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)}.$$

Some special cases of the one-parameter Mittag-Leffler function

$$E_1(-z) = e^{-z}, \quad E_2(-z^2) = \cos z, \quad E_2(z) = e^{z^2} \text{erfc}(-z),$$

where $\text{erfc}(z)$ is the complimentary error function

$$\text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt.$$

The Mittag-Leffler functions appear in the solutions of ordinary and fractional differential equations [2, chap. 1]. The ordinary differential equation

$$y''(x) = y(x), \quad y(0) = 1, \quad y'(0) = 1$$

has solution $y(x) = E_{2,1}(x^2) + x E_{2,2}(x^2) = \cosh x + \sinh x = e^{x}$. The fractional differential equation

$$y^{(\alpha)}(x) = \lambda y(x), \quad y(0) = 1$$

has solution $y(x) = E_{\alpha}(\lambda x^\alpha)$. We can determine the analytical solutions of linear ordinary and partial fractional differential equations using integral transforms. The following formulas for the Laplace transform of the derivatives of the Mittag-Leffler functions are often used to determine the analytical solutions of linear fractional differential equations [2].

$$\mathcal{L}\{t^{\alpha k+\beta-1}E^{(k)}_{\alpha,\beta}(\pm at^\alpha)\}(s) = \frac{k! s^{\alpha-\beta}}{(s^\alpha \mp a)^{\kappa+1}}.$$
Analytical solutions of ordinary and partial fractional differential equations can be found only for special cases of the equations and the initial and boundary conditions. We can determine numerical approximations for the solutions of a much larger class of equations which include nonlinear fractional differential equations. Approximations for the Caputo and Riemann-Liouville derivatives are obtained from the Gr"{u}newald-Letnikov fractional derivative and by approximating the fractional integral in the definition.

Let $x_n = b + nh$ be a uniform grid on the $x$-axis starting from the point $b$, and $y_n = y(x_n) = y(b + nh)$, where $h > 0$ is a small number. The following approximation of the Caputo derivative is derived from quadrature approximations of the fractional integral for $y'(x)$ in the definition of Caputo fractional derivative \([39]\) on the interval $[b, x_n]$, by approximating the integrals on all subintervals of length $h$.

$$y_n^{(\alpha)} = \frac{1}{h^\alpha} \sum_{k=0}^{n-1} c_k^{(\alpha)} y_{n-k} + O(h^{2-\alpha}), \quad (6)$$

where $c_0^{(\alpha)} = 1/\Gamma(2 - \alpha)$ and

$$c_k^{(\alpha)} = \frac{(k + 1)^{1-\alpha} - 2k^{1-\alpha} + (k - 1)^{1-\alpha}}{\Gamma(2 - \alpha)}.$$

When the function $y(x)$ has continuous second derivative, approximation (6) has accuracy $O(h^{2-\alpha})$. The weights $c_k^{(\alpha)}$ satisfy

$$c_0^{(\alpha)} > 0, \quad c_1^{(\alpha)} < c_2^{(\alpha)} < \cdots < c_k^{(\alpha)} < \cdots < 0, \quad \sum_{k=0}^{\infty} c_k^{(\alpha)} = 0.$$

The Gr"{u}newald-Letnikov fractional derivative is closely related to Caputo and Riemann-Liouville derivatives

$$D_{GL}^\alpha y(x) = \lim_{\Delta x \to 0} \frac{1}{\Delta x^\alpha} \sum_{n=0}^{[\Delta x/\Delta x]} (-1)^n \binom{\alpha}{n} y(x - n \Delta x).$$

The two most often used values of the lower limit of the fractional differentiation $b$ are zero and $-\infty$. When the lower limit $b = -\infty$ the upper limit of the sum in the definition of Gr"{u}newald-Letnikov derivative is $\infty$. The fractional binomial coefficients are defined similarly to the integer binomial coefficients with the gamma function

$$\binom{\alpha}{n} = \frac{\Gamma(\alpha + 1)}{\Gamma(n + 1)\Gamma(\alpha - n + 1)} = \frac{\alpha(\alpha - 1)\cdots(\alpha - n + 1)}{n!}.$$
The Riemann-Liouville, Caputo and Grünwald-Letnikov derivatives are equal when \( y(b) = 0 \) and \( y \in C^1[b, x] \) (\([11] \) p. 43). Let’s denote by \( \Delta^\alpha_h y(x) \) and \( \Delta^\alpha_{h,p} y(x) \) the Grünwald difference operator and shifted Grünwald difference operators for the function \( y(x) \).

\[
\Delta^\alpha_h y(x) = \sum_{n=0}^{N_{x,h}} (-1)^n \binom{\alpha}{n} y(x - nh),
\]

\[
\Delta^\alpha_{h,p} y(x) = \sum_{n=0}^{N_{x,h}} (-1)^n \binom{\alpha}{n} y(x - (n - p)h).
\]

where \( N_{x,h} = \left\lfloor \frac{x-b}{h} \right\rfloor \), and \( h > 0 \) is a small number. The Grünwald operator is a special case of the shifted Grünwald operator when the shift value \( p = 0 \). When \( y(b) = 0 \), we derive approximations for the Riemann-Liouville and Caputo derivatives from the definition of Grünwald-Letnikov derivative.

\[
D^\alpha_x y(x) = D^\alpha_{RL} y(x) = D^\alpha_{GL} y(x) \approx h^{-\alpha} \Delta^\alpha_h y(x) \approx h^{-\alpha} \Delta^\alpha_{h,p} y(x).
\]

We will call the approximations \( h^{-\alpha} \Delta^\alpha_h y(x) \) and \( h^{-\alpha} \Delta^\alpha_{h,p} y(x) \) of the fractional derivative of order \( \alpha \) - Grünwald formula and shifted Grünwald formulas of the function \( y(x) \). Let \( w_n^{(\alpha)} \) be the weights of the Grünwald formulas.

\[
w_n^{(\alpha)} = (-1)^n \binom{\alpha}{n}.
\]

When \( y(x) \) is a continuously-differentiable function the shifted Grünwald formulas for the function \( y(x) - y(b) \) are first-order approximations for the Caputo derivative of \( y(x) \).

\[
y^{(\alpha)}(x) = \frac{1}{h^\alpha} \sum_{n=0}^{N_{x,h}} w_n^{(\alpha)} (y(x - (n - p)h) - y(b)) + O(h).
\] (7)

In Theorem 1(i) we show that the shifted Grünwald formulas of the function \( y(x) - y(b) \) are second-order approximations for the Caputo fractional derivative at the point \( x + (p - \alpha/2)h \), when the function \( y(x) \) is sufficiently differentiable on the interval \([b, x]\) and the values of its first and second derivatives are equal to zero at the point \( b \).

\[
y^{(\alpha)} \left( x + \left( p - \frac{\alpha}{2} \right) h \right) = \frac{1}{h^\alpha} \sum_{n=0}^{N_{x,h}} w_n^{(\alpha)} (y(x - (n - p)h) - y(b)) + O(h^2).
\] (8)
We derive the above formula in Theorem 1(i) from relation (13) for the shifted Gr"{u}newald formulas and the fractional derivatives of the function $y(x)$. When the conditions of Theorem 1 are satisfied the Riemann-Liouville and Caputo derivatives are equal. The values of a function and the shifted Gr"{u}newald formulas satisfy

$$\beta_1 y(x_1) + \beta_2 y(x_2) = y(\beta_1 x_1 + \beta_2 x_2) + O\left(h^2\right),$$

$$\beta_1 \Delta_{h,p}^\alpha y(x_1) + \beta_2 \Delta_{h,q}^\alpha y(x_2) = \Delta_{h,\beta_1 p + \beta_2 q}^\alpha y(\beta_1 x_1 + \beta_2 x_2) + O\left(h^2\right).$$

when $\beta_1 + \beta_2 = 1$ and $y(x)$ is a sufficiently smooth function. An alternative way to obtain (13) is to apply the approximation for average value of shifted Grunwald formulas to approximation (2.15) in Tian et al. [30]. An important special case of the above formula is when $y(b) = 0$ and $p = 0$.

$$y^{(\alpha)}\left(x - \frac{\alpha h}{2}\right) = \frac{1}{h^\alpha} \sum_{n=0}^{N_x,h} w_n^{(\alpha)} y(x - nh) + O\left(h^2\right). \quad (9)$$

This approximation is closely related to formula (2.9) in [25] and is suitable for constructing second order weighted numerical approximations for fractional differential equations on a uniform grid. As a direct consequence of (9) we obtain a second order approximation for the Gr"{u}newald formula using average values of Caputo derivatives on consecutive nodes of a uniform grid.

$$\frac{1}{h^\alpha} \sum_{n=0}^{N_x,h} w_n^{(\alpha)} y(x - nh) = \left(\frac{\alpha}{2}\right) y_{n-1}^{(\alpha)} + \left(1 - \frac{\alpha}{2}\right) y_n^{(\alpha)} + O\left(h^2\right). \quad (10)$$

In Corollary 5 we determine a third order approximation for the Gr"{u}newald formula using a weighted average of three consecutive values of the Caputo derivative on a uniform grid, for sufficiently differentiable functions $y(x)$ which satisfy the conditions of Theorem 1(ii).

$$\frac{1}{h^\alpha} \sum_{n=0}^{N_x,h} w_n^{(\alpha)} y(x - nh) = \left(\frac{a^2}{8} - \frac{5a}{24}\right) y_{n-2}^{(\alpha)} + \left(\frac{11a}{12} - \frac{a^2}{4}\right) y_{n-1}^{(\alpha)} + \left(1 - \frac{17a}{24} + \frac{a^2}{8}\right) y_n^{(\alpha)} + O\left(h^3\right). \quad (11)$$

Approximations (9), (10) and (11) are suitable for numerical computations for fractional differential equations on a uniform grid, when the solutions are sufficiently differentiable functions. In section 4 we determine second and third order approximations for ordinary differential equation (2), and in
section 5 we construct stable difference approximations for the fractional sub-
diffusion equation which have second order accuracy with respect to the space
and time variables. The Gr"{u}newald weights $w_n^{(\alpha)}$ are computed recursively
with $w_0^{(\alpha)} = 1$, $w_1^{(\alpha)} = -\alpha$ and
\[ w_n^{(\alpha)} = \left(1 - \frac{\alpha + 1}{n}\right) w_{n-1}^{(\alpha)}. \]
The numbers $w_n^{(\alpha)}$ are the coefficients of the binomial series
\[ (1 - z)^\alpha = \sum_{n=0}^{\infty} w_n^{(\alpha)} z^n. \]
When $\alpha$ is a positive integer the sum is finite, and the binomial series con-
verges at the point $z = 1$ when $0 < \alpha < 1$. The weights $w_n^{(\alpha)}$ have the
following properties.
\[ w_0^{(\alpha)} > 0, \quad w_1^{(\alpha)} < w_2^{(\alpha)} < \cdots < w_n^{(\alpha)} < \cdots < 0, \quad \sum_{n=0}^{\infty} w_n^{(\alpha)} = 0. \tag{12} \]
When the lower limit of fractional differentiation $b \neq \infty$, the upper limit of
the sum is finite and $\sum_{n=0}^{N_{x,h}} w_n^{(\alpha)} > 0$. The shifted Gr"{u}newald formulas for
$y(x)$ are first order approximations for the Riemann-Liouville derivative of
the function $y(x)$. The approximation error can be represented as a sum of
higher order Riemann-Liouville fractional derivatives \[13\]. This estimate is
obtained in Tadjeran et al. \[23\] when the order $\alpha$ of the Riemann-Liouville
derivative is between one and two using Fourier transform of the shifted
Gr"{u}newald formulas. The estimate for the error of the shifted Gr"{u}newald
formulas is generalized in Hejazi et al. \[26\] for arbitrary positive $\alpha$ and $p$.

**Theorem.** Let $\alpha$ and $p$ be positive numbers, and suppose that $y \in C^{[\alpha]+n+2}(\mathbb{R})$
and all derivatives of $y$ up to order $[\alpha] + n + 2$ belong to $L^1(\mathbb{R})$. Then if
$b = -\infty$, there exist constants $c_l$ independent of $h, y, x$ such that
\[ h^{-\alpha} \Delta_{b,p} y(x) = D_{RL}^\alpha y(x) + \sum_{l=1}^{n-1} c_l h^l D_{RL}^{\alpha+l} y(x) + O(h^n). \tag{13} \]
The numbers $c_l$ are the coefficients of the series expansion of the function
\[ \omega_{\alpha,p}(z) = \left(1 - e^{-z}\right)^{\alpha} e^{pz}. \]
If a function $y(x)$ is defined on a finite interval $I$ we can extend it to the real
line by setting $y(x) = 0$ when $x \notin I$. In this way the Caputo derivative of
the extended function is equal to zero when $x \notin \mathcal{I}$. In the next section we use (13) to determine second and third order approximations for the Grünwald and shifted Grünwald formulas with weighted averages of Caputo derivatives on consecutive points of a uniform grid.

3 Approximations for Grünwald and shifted Grünwald formulas

The definitions of Riemann-Liouville and Caputo derivatives are the two most commonly used definitions for fractional derivatives. The Caputo and Riemann-Liouville fractional derivatives of order $n + \alpha$, where $n$ is a positive integer and $0 < \alpha < 1$ are defined as

$$D_{x}^{n+\alpha}y(x) = \frac{1}{\Gamma(1-\alpha)} \int_{b}^{x} \frac{y^{(n+1)}(\xi)}{(x-\xi)^{\alpha}} d\xi,$$

$$D_{RL}^{n+\alpha}y(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d^{n+1}}{dx^{n+1}} \int_{b}^{x} \frac{y(\xi)}{(x-\xi)^{\alpha}} d\xi.$$

When $y(x)$ is sufficiently differentiable function on the interval $[b, x]$, the Riemann-Liouville and Caputo derivatives are related as [1, p. 53]

$$D_{RL}^{n+\alpha}y(x) = D_{x}^{n+\alpha}y(x) + \sum_{k=0}^{n} \frac{y^{(k)}(b)}{\Gamma(k-\alpha-1)(x-b)^{k-\alpha-n}}.$$

We can compute the value of the Riemann-Louville derivative of the function $y(x)$ from the value of the Caputo derivative and its integer order derivatives at the lower limit $b$. One disadvantage of the Riemann-Liouville derivative is that it has a singularity at the lower limit $b$. When $\alpha > 1$ the singularity is non-integrable. The class of Caputo differentiable functions of order $n + \alpha$ includes the functions with $n + 1$ continuous derivatives. In section 2 we discussed properties of the Caputo derivatives at the lower limit $b$, which are related to the properties of the integer order derivatives. We often prefer to study fractional differential equations with the Caputo derivative because its properties make it an attractive fractional derivative for numerical solution of fractional differential equations. Let $h$ be the step size of a uniform grid on the $x$-axis starting from the lower limit of fractional differentiation $b$ and

$$x_{n} = b + nh, \quad y_{n} = y(x_{n}) = y(b + nh).$$

In Theorem 1 we use the estimate for the error of the shifted Grünwald formulas (13) and relation (14) for the Riemann-Liouville and Caputo derivatives to obtain second and third order approximations for the shifted Grünwald formulas using fractional order Caputo and Miller-Ross derivatives.
Theorem 1. (Approximations for the shifted Grünwald formulas)

(i) Let $y(b) = y'(b) = y''(b) = 0$ and $y \in C^4[b, x]$. Then

$$h^{-\alpha} \Delta_{h,p}^\alpha y(x) = y^{(\alpha)}(x) \left(x + \left(p - \frac{\alpha}{2}\right) h\right) + O\left(h^2\right); \quad (15)$$

(ii) Let $y(0) = y'(0) = y''(0) = y'''(0) = y''''(b) = 0$ and $y \in C^5[b, x]$. Then

$$h^{-\alpha} \Delta_{h,p}^\alpha y(x) = y^{(\alpha)}(x) \left(x + \left(p - \frac{\alpha}{2}\right) h\right) + \frac{\alpha}{24} h^2 y^{(2+\alpha)}(x) + O\left(h^3\right).$$

Proof. The function $\omega_{\alpha,p}(z)$ has power series expansion

$$\omega_{\alpha,p}(z) = \left(\frac{1-e^{-z}}{z}\right)^\alpha e^{pz} = c_0 + c_1 z + c_2 z^2 + \cdots,$$

where $c_0 = 1$, $c_1 = p - \alpha/2$ and $c_2 = \frac{1}{24}(12p^2 - 12\alpha p + \alpha + 3\alpha^2) - \frac{1}{24} \left(p^2 - \alpha p + \frac{\alpha^2}{4}\right) = \frac{\alpha}{24} + \frac{1}{2} \left(p - \frac{\alpha}{2}\right)^2$.

From (13) and $n = 2$ we obtain

$$h^{-\alpha} \Delta_{h,p}^\alpha y(x) = D_{RL}^\alpha y(x) + \left(p - \frac{\alpha}{2}\right) h D_{RL}^{\alpha+1} y(x) + O\left(h^2\right).$$

Let $0 < \beta < 1$. The Caputo and Riemann-Liouville fractional derivatives of order $3 + \beta$ satisfy (14) with $n = 3$. The Riemann-Liouville derivative $D_{RL}^{3+\beta} y(x)$ has non-integrable singularities of orders $1+\beta, 2+\beta$ and $3+\beta$ at the lower limit $b$, with coefficients $y(b)$, $y'(b)$ and $y''(b)$. The Caputo derivative of $y(x)$ of order $3+\beta$ and the function $(x-b)^{-\beta}$ are integrable on a finite interval. Therefore $D_{RL}^{3+\beta} y(x) \in L^1[b, x]$ when $y(b) = y'(b) = y''(b) = 0$. Similarly, $D_{RL}^{4+\beta} y(x) \in L^1[b, x]$ when $y(b) = y'(b) = y''(b) = y'''(b) = 0$.

The Riemann-Liouville and Caputo derivatives of order $\alpha$ for the functions $y(x)$ which satisfy the conditions of Theorem 1 are equal

$$D_{RL}^\alpha y(x) = y^{(\alpha)}(x)$$

and we can represent $D_{RL}^{\alpha+1} y(x)$ with the Caputo derivative $y^{(\alpha)}(x)$ as

$$D_{RL}^{\alpha+1} y(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d^2}{dx^2} \int_b^x \frac{y(\xi)}{(x-\xi)^\alpha} d\xi = \frac{d}{dx} D_{RL}^\alpha y(x) = \frac{d}{dx} y^{(\alpha)}(x).$$

We obtain the following relation for the shifted Grünwald formulas and the Caputo derivative of the function $y(x)$.

$$h^{-\alpha} \Delta_{h,p}^\alpha y(x) = y^{(\alpha)}(x) + \left(p - \frac{\alpha}{2}\right) h \frac{d}{dx} y^{(\alpha)}(x) + O\left(h^2\right).$$
From the mean value theorem for the function \( y^{(\alpha)}(x) \) we have that
\[
y^{(\alpha)}\left( x + \left( p - \frac{\alpha}{2} \right) h \right) = y^{(\alpha)}(x) + \left( p - \frac{\alpha}{2} \right) h \frac{d}{dx} y^{(\alpha)}(x) + O(h^2).
\]
Therefore
\[
y^{(\alpha)}\left( x + \left( p - \frac{\alpha}{2} \right) h \right) = h^{-\alpha} \Delta^{\alpha}_{h,p} y(x) + O(h^2).
\]

Now we prove (ii). From (13) and \( n = 3 \) we obtain
\[
h^{-\alpha} \Delta^{\alpha}_{h,p} y(x) = D^{\alpha}_{RL} y(x) + \left( p - \frac{\alpha}{2} \right) h D^{\alpha+1}_{RL} y(x) + \left( \frac{\alpha}{24} + \frac{1}{2} \left( p - \frac{\alpha}{2} \right)^2 \right) h^2 D^{2+\alpha}_{RL} y(x) + O(h^3).
\]
We have that
\[
D^{2+\alpha}_{RL} y(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d^3}{dx^3} \int_b^x \frac{y(\xi)}{(x-\xi)\alpha} d\xi = \frac{d^2}{dx^2} D^{\alpha}_{RL} y(x) = \frac{d^2}{dx^2} y^{(\alpha)}(x).
\]
Then
\[
h^{-\alpha} \Delta^{\alpha}_{h,p} y(x) = y^{(\alpha)}(x) + \left( p - \frac{\alpha}{2} \right) h \frac{d}{dx} y^{(\alpha)}(x) + \frac{1}{2} \left( p - \frac{\alpha}{2} \right)^2 h^2 \frac{d^2}{dx^2} y^{(\alpha)}(x) + \frac{\alpha}{24} h^2 \frac{d^2}{dx^2} y^{(\alpha)}(x) + O(h^3).
\]
From the Mean-Value Theorem for \( y^{(\alpha)}(x) \) we obtain
\[
h^{-\alpha} \Delta^{\alpha}_{h,p} y(x) = y^{(\alpha)}\left( x + \left( p - \frac{\alpha}{2} \right) h \right) + \frac{\alpha}{24} h^2 y^{(2+\alpha)} + O(h^3).
\]

The most useful special case of (13) is when \( p = 0 \).

**Corollary 2.** Let \( y(b) = y'(b) = y''(b) = 0 \) and \( y \in C^4[b, x] \). Then
\[
h^{-\alpha} \Delta^{\alpha}_{h} y(x) = y^{(\alpha)}\left( x - \frac{\alpha h}{2} \right) + O(h^2).
\]
(16)

When \( \alpha = 1 \) and \( \alpha = 2 \) approximation (16) becomes a central difference approximation for the first and second derivatives of the function \( y(x) \)
\[
y'\left( x - \frac{h}{2} \right) = \frac{y(x) - y(x-h)}{h} + O(h^2),
\]
Hence, to the proof of (17).

The proof for approximation (18) uses third order expansions and is similar to Lemma 4.

Lemma 4. (Approximations for the shifted Grünwald formulas)

(i) Let \( y(b) = y'(b) = y''(b) = 0 \) and \( y \in C^4[b, x] \). Then

\[
h^{-\alpha} \Delta_h^{\alpha} y_n = \left( \frac{\alpha}{2} - p \right) y_n^{(\alpha)} + \left( 1 + p - \frac{\alpha}{2} \right) y_{n-1}^{(\alpha)} + O \left( h^2 \right);
\]

(ii) Let \( y(b) = y'(b) = y''(b) = y'''(b) = 0 \) and \( y \in C^5[b, x] \). Then

\[
h^{-\alpha} \Delta_h^{\alpha} y_n = \overline{\beta}_1 y_{n-2}^{(\alpha)} + \overline{\beta}_2 y_{n-1}^{(\alpha)} + \overline{\beta}_3 y_n^{(\alpha)} + O \left( h^3 \right),
\]

where \( \overline{\beta}_1 = \frac{p}{2} + \frac{p^2}{2} - \frac{5\alpha}{24} - \frac{p\alpha}{2} + \frac{\alpha^2}{8} \) and

\[
\overline{\beta}_2 = -2p - p^2 + \frac{11\alpha}{12} + p\alpha - \frac{\alpha^2}{4}, \quad \overline{\beta}_3 = 1 + \frac{3p}{2} + \frac{p^2}{2} - \frac{17\alpha}{24} - \frac{p\alpha}{2} + \frac{\alpha^2}{8}.
\]
Proof. From Theorem 1(i) with \(x = x_n\) we have
\[ h^{-\alpha} \Delta_{h,p}^{\alpha} y_n = y^{(\alpha)} \left(x_n + \left(p - \frac{\alpha}{2}\right) h\right) + O(h^2). \]

From (17) with \(\beta = \frac{\alpha}{2} - p\) we obtain
\[ h^{-\alpha} \Delta_{h,p}^{\alpha} y_n = \left(\frac{\alpha}{2} - p\right) y_{n-1}^{(\alpha)} + \left(1 + p - \frac{\alpha}{2}\right) y_n^{(\alpha)} + O(h^2). \]

Now we use the formula from Theorem 1(ii) to determine a third order approximation for the shifted Grünwald formulas.
\[ h^{-\alpha} \Delta_{h,p}^{\alpha} y_n = y^{(\alpha)} \left(x_n + \left(p - \frac{\alpha}{2}\right) h\right) + \frac{\alpha h^2}{24} y_n^{(2+\alpha)} + O(h^3). \]

The central difference approximation for \(y_{n-1}^{(\alpha)}\) with nodes \(\{x_{n-2}, x_{n-1}, x_n\}\) has order \(O(h)\)
\[ y_{n-1}^{(2+\alpha)} = \frac{y_n^{(\alpha)} - 2y_{n-1}^{(\alpha)} + y_{n-2}^{(\alpha)}}{h^2} + O(h), \]

Then
\[ h^{-\alpha} \Delta_{h,p}^{\alpha} y_n = y^{(\alpha)} \left(x_n + \left(p - \frac{\alpha}{2}\right) h\right) + \frac{\alpha h^2}{24} \left(\frac{y_n^{(\alpha)} - 2y_{n-1}^{(\alpha)} + y_{n-2}^{(\alpha)}}{h^2} + O(h)\right) + O(h^3). \]

From (18) with \(\beta = \frac{\alpha}{2} - p\) we obtain approximation (20).

We obtain second and third order approximations for the Grünwald formula from (19) and (20) with \(p = 0\).

**Corollary 5.** (Approximations for the Grünwald formula)

(i) Let \(y(b) = y'(b) = y''(b) = 0\) and \(y \in C^4[b, x]\). Then
\[ h^{-\alpha} \Delta_{h}^{\alpha} y_n = \left(\frac{\alpha}{2}\right) y_{n-1}^{(\alpha)} + \left(1 - \frac{\alpha}{2}\right) y_n^{(\alpha)} + O(h^2); \]

(ii) Let \(y(b) = y'(b) = y''(b) = y'''(b) = 0\) and \(y \in C^5[b, x]\). Then
\[ h^{-\alpha} \Delta_{h}^{\alpha} y_n = \left(\frac{a^2}{8} - \frac{5a}{24}\right) y_{n-2}^{(\alpha)} + \left(\frac{11a}{12} - \frac{a^2}{4}\right) y_{n-1}^{(\alpha)} + \left(1 - \frac{17a}{24} + \frac{a^2}{8}\right) y_n^{(\alpha)} + O(h^3). \]

In Corollary 2 and Corollary 5 we determined second and third order approximations for the Grünwald formula using values of Caputo derivatives. The three approximations are suitable for algorithms for numerical solution of fractional differential equations on a uniform grid. In the next lemma, we discuss a property of the Caputo derivative of a continuously differentiable function in a neighborhood of the lower limit \(b\).
Lemma 6. Let $0 < \alpha < 1$ and $y \in C^1[b, b + \epsilon]$, where $\epsilon > 0$. Then

$$y^{(\alpha)}(b) = 0.$$ 

Proof. The function $y'$ is bounded on the interval $[b, b + \epsilon]$. Let

$$\delta = \max_{b \leq x \leq b + \epsilon} y'(x).$$

When $b < x < b + \epsilon$ we have

$$|y^{(\alpha)}(x)| \leq \frac{1}{\Gamma(1 - \alpha)} \int_b^x \frac{|y'(|\xi|)|}{(x - \xi)^\alpha} d\xi \leq \frac{\delta}{\Gamma(1 - \alpha)} \int_b^x (x - \xi)^{-\alpha} d\xi,$$

$$|y^{(\alpha)}(x)| \leq \frac{\delta}{\Gamma(1 - \alpha)} \frac{(x - \xi)^{1-\alpha}}{1 - \alpha} \bigg|_b^x \leq \frac{\delta(x - b)^{1-\alpha}}{\Gamma(2 - \alpha)}.$$

From the squeeze low of limits

$$0 \leq \lim_{x \downarrow b} |y^{(\alpha)}(x)| \leq \lim_{x \downarrow b} \frac{\delta(x - b)^{1-\alpha}}{\Gamma(2 - \alpha)} = 0.$$ 

Hence,

$$y^{(\alpha)}(b) = \lim_{x \downarrow b} y^{(\alpha)}(x) = 0.$$

In the next two sections we compute approximations for the solutions of equations (1) and (2) when $b = 0$ and the solutions are sufficiently differentiable functions. We use the result from Lemma 6 to determine the values of the derivatives of the solution of equation (2) at the lower limit $x = 0$, and the partial derivatives $u_t(x, 0)$ and $u_{tt}(x, 0)$ of the solution of the fractional sub-diffusion equation (1) when $t = 0$.

4 Numerical solution of ordinary fractional differential equations

The field of numerical computations for fractional differential equations has been rapidly gaining popularity for the last several decades. The fractional differential equations have diverse algorithms for computation of numerical solutions and a potential for practical applications. The analytical solutions of linear fractional differential equations with constant coefficients are determined with the integral transforms method [2]. The algorithms for numerical solution can be used for a much larger class of equations including fractional differential equations with non-constant coefficients. Dithelm et al. [60] proposed a prediction-correction algorithm for numerical approximation
for ordinary fractional differential equations with accuracy $O \left( h^{\min\{2,1+\alpha\}} \right)$. Deng [63] presented an improved prediction-correction algorithm with accuracy $O \left( h^{\min\{2,1+2\alpha\}} \right)$. Higher order prediction-correction algorithms are discussed in [37]. While the number of computations for numerical solution of ordinary fractional differential equations is much smaller than the number of computations for partial fractional differential equations it is greater than the number of computations for ordinary differential equations. An acceptable approximation (22) for the solution of equation (2) is obtained from the Grünwald formula approximation for the Caputo derivative. It converges to the exact solution with accuracy $O(h)$. An improved approximation (23) with accuracy $O(h^{2-\alpha})$ is obtained when we use approximation (6) instead of the Grünwald formula. Numerical experiments for equation (24) and approximations (22) and (23) on the interval $[0,1]$ are given in Table 1. In Figure 1 the two approximations are compared with the exact solution and the second order approximation (25), when $h = 0.1$.

In the present section we use approximations (10) and (11) to obtain recurrence relations for second and third order approximations to the solution of ordinary fractional differential equation (2) on the interval $[0,1]$, 

$$y^{(\alpha)}(x) + y(x) = f(x)$$

and we give a proof for the convergence of the algorithm. We can assume that equation (2) has initial condition

$$y(0) = 0$$

because the function $\overline{y}(x) = y(x) - y(0)$ is a solution of equation (2) with right-hand side $\overline{f}(x) = f(x) - y(0)$. The exact solution of equation (2) is obtained with the Laplace transform method [2],

$$y(x) = \int_{0}^{x} \xi^{\alpha-1} E_{\alpha,\alpha} \left( -\xi^{\alpha} \right) f(x - \xi) d\xi.$$ 

An alternative approach to nonzero initial condition is to use approximations (9), (10) and (11) for the function $y(x) - y(0)$ (as in formulas (7) and (8)).

Let $h = T/N$ where $T > 0$ and $N$ is a positive integer. By approximating the fractional derivative at the point $x_n = nh$ using the Grünwald formula we obtain

$$\frac{1}{h^{\alpha}} \sum_{k=0}^{n} w_k^{(\alpha)} y_n - k + y_n \approx f_n,$$

$$y_n + \sum_{k=1}^{n} w_k^{(\alpha)} y_{n-k} + h^{\alpha} y_n \approx h^{\alpha} f_n.$$
Table 1: Maximum error and order of approximations (22) and (23) for equation (24) on the interval [0, 1] when $\alpha = 2/3$.

| $h$  | Error       | Order  | $h$  | Error       | Order  |
|------|-------------|--------|------|-------------|--------|
| 0.05 | 0.0560953   | 0.991369 | 0.05 | 0.0223527   | 1.28672 |
| 0.025| 0.0281318   | 0.995677 | 0.025| 0.0090448   | 1.30529 |
| 0.0125| 0.0140870  | 0.997837 | 0.0125| 0.0036319   | 1.31636 |
| 0.00625| 0.0070488  | 0.998918 | 0.00625| 0.0014517   | 1.32299 |
| 0.003125| 0.0035257 | 0.999459 | 0.003125| 0.0005786   | 1.32699 |

The truncation errors of the two approximations are $O(h)$ and $O(h^{1+\alpha})$. We compute an approximation $\tilde{y}_n$ to the exact solution of (2) at the point $x_n$ with $\tilde{y}_0 = 0$ and the recurrence relations

$$\tilde{y}_n = \frac{1}{1 + h^\alpha} \left( h^n f_n - \sum_{k=1}^{n} w_k^{(\alpha)} \tilde{y}_{n-k} \right). \quad (22)$$

Approximation (22) has accuracy $O(h)$. By approximating at the Caputo derivative at the points $x_n$ with (6) we obtain similar recurrence relations

$$\tilde{y}_n = \frac{1}{h^\alpha + c_0^{(\alpha)}} \left( h^n f_n - \sum_{k=1}^{n} c_k^{(\alpha)} \tilde{y}_{n-k} \right). \quad (23)$$

The accuracy of approximation (23) is $O(h^{2-\alpha})$. We evaluate numerically the performance of approximations (22) and (23) for the equation

$$y^{(\alpha)}(x) + y(x) = 2x^{2+\alpha} + \Gamma(3 + \alpha)x^2. \quad (24)$$

Equation (24) has solution $y(x) = 2x^{2+\alpha}$. When $h = 0.1$ and $\alpha = 2/3$ the maximum error of approximations (22) and (23) are 0.111521 and 0.0545347. In Table 1 we compute the maximum errors and the order of approximations (22) and (23) for $\alpha = 2/3$ and different values of $h$. The graphs of approximations (22) and (23) (filled squares and empty circles) and the solution of (24) on the interval [0, 1] are given in Figure 1.

### 4.1 Second-order approximations

In Corollary 5 we determined a second order approximation (10) for the Grünwald formula with average values of Caputo derivatives. We use the approximation and (17) to obtain second order numerical solutions (25) and (26) for equation (2).

$$h^{-\alpha} \Delta_h^\alpha y_n = \left( \frac{\alpha}{2} \right) y_n^{(\alpha)} + \left( 1 - \frac{\alpha}{2} \right) y_{n-1}^{(\alpha)} + O(h^2). \quad (25)$$
From equation (2) we have
\[ y_{n-1}^{(\alpha)} = f_{n-1} - y_{n-1}, \quad y_n^{(\alpha)} = f_n - y_n. \]

Then
\[ \Delta_h^\alpha y_n = h^\alpha \left( \frac{\alpha}{2} \right) (f_{n-1} - y_{n-1}) + h^\alpha \left( 1 - \frac{\alpha}{2} \right) (f_n - y_n) + O(h^{2+\alpha}). \]

The Grünwald formula for \( y_n \) is defined as
\[ \Delta_h^\alpha y_n = \sum_{k=0}^{n} w_k^{(\alpha)} y_{n-k} = y_n + \sum_{k=1}^{n} w_k^{(\alpha)} y_{n-k}. \]

Let
\[ \gamma = \frac{1}{1 + h^\alpha \left( 1 - \frac{\alpha}{2} \right)}. \]

The exact solution of equation (2) satisfies
\[ y_n = \gamma \left( h^\alpha \left( \frac{\alpha}{2} \right) (f_{n-1} - y_{n-1}) + h^\alpha \left( 1 - \frac{\alpha}{2} \right) f_n - \sum_{k=1}^{n} w_k^{(\alpha)} y_{n-k} \right) + O(h^{2+\alpha}). \]

We can obtain a more convenient form of the above formula using (17)
\[ f_{n-1}^{\alpha} = \left( \frac{\alpha}{2} \right) f_{n-1} + \left( 1 - \frac{\alpha}{2} \right) f_n + O(h^2), \]
\[ y_n = \frac{1}{1 + \left( 1 - \frac{\alpha}{2} \right) h^\alpha} \left( h^\alpha f_{n-1}^{\alpha} + \frac{\alpha}{2} (2 - h^\alpha) y_{n-1} - \sum_{k=2}^{n} w_k^{(\alpha)} y_{n-k} \right) + O(h^{2+\alpha}). \]

We compute second order approximations \( \bar{y}_n \) to the exact solution \( y_n \) of equation (2) with \( \bar{y}_0 = 0 \) and the recurrence relations
\[ \bar{y}_n = \frac{1}{1 + \left( 1 - \frac{\alpha}{2} \right) h^\alpha} \left( h^\alpha f_{n-1}^{\alpha} + \frac{\alpha}{2} (2 - h^\alpha) \bar{y}_{n-1} - \sum_{k=2}^{n} w_k^{(\alpha)} \bar{y}_{n-k} \right), \quad (25) \]
\[ \bar{y}_n = \gamma \left( h^\alpha \left( 1 - \frac{\alpha}{2} \right) f_n + \frac{\alpha}{2} f_{n-1} + \frac{\alpha}{2} (2 - h^\alpha) \bar{y}_{n-1} - \sum_{k=2}^{n} w_k^{(\alpha)} \bar{y}_{n-k} \right). \quad (26) \]
Theorem 7. Suppose that the solution $y(x)$ of equation (2) is sufficiently differentiable function on an interval $[0, T]$ and

$$y(0) = y'(0) = y''(0) = 0.$$  

Then approximations (25) and (26) converge to the solution of equation (2) with accuracy $O(h^2)$.

The proof of Theorem 7 is similar to the proof of Theorem 14. The two numerical solutions (25) and (26) have second order accuracy $O(h^2)$. Experimental results suggest that in many cases the error of approximation (25) is smaller than the error of approximation (26) because it has a smaller truncation error. In Table 2 we compute the maximum error and order of approximation (25) for equation (24) and different values of $h$. When $h = 0.1$ and $\alpha = 2/3$ the error of approximation (25) is 0.005828. In Figure 2 we compare approximations (22), (23) and (25) with the exact solution of equation (24).

Figure 1: Graph of the exact solution of equation (24) and approximations (22), (23) and (25) for $h = 0.1$ and $\alpha = 2/3$.

Suppose that the solution $y(x)$ of equation (2) is sufficiently differentiable function. Denote

$$L_1 = y'(0), \quad L_2 = y''(0), \quad L_3 = y'''(0).$$

In the next lemma we determine $L_1$ and $L_2$ from the function $f(x)$.

Lemma 8. Suppose that $y(x)$ is a sufficiently differentiable solution of (2).

$$f(0) = 0, \quad L_1 = \lim_{x \to 0} f^{(1-\alpha)}(x),$$

$$L_2 = \lim_{x \to 0} \left( \frac{d}{dx} f^{(1-\alpha)}(x) - \frac{L_1 x^{-\alpha}}{\Gamma(\alpha)} \right).$$
Table 2: Maximum error and order of approximation (25) for equation (24) on the interval \([0, 1]\) and \(\alpha = 2/3\).

| \(h\)  | \(Error\)    | \(Ratio\)    | \(\log_2(Ratio)\) |
|--------|--------------|--------------|------------------|
| 0.05   | 0.00146501   | 3.97836      | 1.99217          |
| 0.025  | 0.00036724   | 3.98921      | 1.99610          |
| 0.0125 | 0.00009193   | 3.99461      | 1.99805          |
| 0.00625| 0.00002210   | 3.99731      | 1.99903          |
| 0.003125| 5.75 \times 10^{-6}  | 3.99865      | 1.99951          |

\[\begin{array}{cccc}
\hline
h & Error & Ratio & \log_2(Ratio) \\
\hline
0.05 & 0.00146501 & 3.97836 & 1.99217 \\
0.025 & 0.00036724 & 3.98921 & 1.99610 \\
0.0125 & 0.00009193 & 3.99461 & 1.99805 \\
0.00625 & 0.00002210 & 3.99731 & 1.99903 \\
0.003125 & 5.75 \times 10^{-6} & 3.99865 & 1.99951 \\
\end{array}\]

\textbf{Proof.} From Lemma 6 we have that
\[y^{(\alpha)}(0) = 0, \quad \text{and} \quad y^{(1-\alpha)}(0) = 0.\]

Then
\[0 = y(0) = f(0) - y^{(\alpha)}(0) = f(0).\]

By applying fractional differentiation of order \(1-\alpha\) to both sides of (2)
\[y'(x) + y^{(1-\alpha)}(x) = f^{(1-\alpha)}(x).\]

Hence,
\[L_1 = y'(0) = f^{(1-\alpha)}(0) - y^{(1-\alpha)}(0) = f^{(1-\alpha)}(0) = \lim_{x \downarrow 0} f^{(1-\alpha)}(x).\]

By differentiating equation (2) we obtain
\[y''(x) + y^{(1+(1-\alpha))}(x) = f^{(1+(1-\alpha))}(x).\]

We determine the value of the Miller-Ross derivative \(y^{(1+(1-\alpha))}(0)\) using differentiation and integration by parts.
\[y^{(1+(1-\alpha))}(x) = \frac{d}{dx}y^{(1-\alpha)}(x) = \frac{1}{\Gamma(\alpha)} \frac{d}{dx} \left( \int_0^x \frac{y'(\xi)}{(x-\xi)^{1-\alpha}} d\xi \right),\]
\[\Gamma(\alpha)y^{(1+(1-\alpha))}(x) = -\frac{d}{dx} \left( \int_0^x y'(\xi)d\frac{(x-\xi)^\alpha}{\alpha} \right),\]
\[\Gamma(1+\alpha)y^{(1+(1-\alpha))}(x) = -\frac{d}{dx} \left( y'(\xi)(x-\xi)^\alpha \right) \bigg|_0^x - \int_0^x y''(\xi)(x-\xi)^\alpha d\xi,\]
\[\Gamma(1+\alpha)y^{(1+(1-\alpha))}(x) = -\frac{d}{dx} \left( -y'(0)x^\alpha - \int_0^x y''(\xi)(x-\xi)^\alpha d\xi \right),\]
\[ y^{(1+(1-\alpha))}(x) = y'(0)x^{\alpha-1} + \frac{1}{\Gamma(\alpha)} \int_0^x \frac{y''(\xi)}{(x-\xi)^{1-\alpha}} d\xi, \quad (28) \]

\[ y^{(1+(1-\alpha))}(x) = \frac{y'(0)x^{\alpha-1}}{\Gamma(\alpha)} + D_x^{2-\alpha}y(x). \]

From (27),

\[ y''(x) = f^{(1+(1-\alpha))}(x) - \frac{L_1x^{\alpha-1}}{\Gamma(\alpha)} - D_x^{2-\alpha}y(x). \]

We have that \( D_x^{2-\alpha}y(0) = 0 \), when \( y \in C^2[0,1] \). Hence,

\[ L_2 = y''(0) = \lim_{x \to 0} \left( f^{(1+(1-\alpha))}(x) - \frac{L_1x^{\alpha-1}}{\Gamma(\alpha)} \right). \]

Let

\[ z(x) = y(x) - L_1x - \frac{L_2}{2}x^2. \quad (29) \]

**Lemma 9.** The function \( z(x) \) satisfies \( z(0) = z'(0) = z''(0) = 0 \) and is a solution of the ordinary fractional differential equation

\[ z^{(\alpha)}(x) + z(x) = F(x), \quad (30) \]

where

\[ F(x) = f(x) - L_1x - \frac{L_2}{2}x^2 - \frac{L_1}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{L_2}{\Gamma(3-\alpha)}x^{2-\alpha}. \]

**Proof.** \( z(0) = y(0) = 0 \). By differentiating (29)

\[ z'(0) = y'(0) - L_1 = 0, \quad z''(0) = y''(0) - L_2 = 0. \]

The function \( z(x) \) has fractional derivative of order \( \alpha \)

\[ z^{(\alpha)}(x) = y^{(\alpha)}(x) - \frac{L_1}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{L_2}{\Gamma(3-\alpha)}x^{2-\alpha}. \]

Then

\[ z^{(\alpha)}(x) + z(x) = y^{(\alpha)}(x) + y(x) - L_1x - \frac{L_2}{2}x^2 - \frac{L_1}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{L_2}{\Gamma(3-\alpha)}x^{2-\alpha}; \]

\[ z^{(\alpha)}(x) + z(x) = f(x) - L_1x - \frac{L_2}{2}x^2 - \frac{L_1}{\Gamma(2-\alpha)}x^{1-\alpha} - \frac{L_2}{\Gamma(3-\alpha)}x^{2-\alpha}. \]

Approximations (25) and (26) are second order numerical solutions of equation (30), because the function \( z(x) \) satisfies the conditions of Lemma 7.
4.2 Estimates for Grünwald weights

In section 4.1 we determined recurrence relations (25) and (26) for second order numerical solutions of equation (2). In section 4.3 and section 5 we obtain a third order numerical solution of equation (2) and second order difference approximations for the fractional sub-diffusion equation. In Theorem 7, Theorem 14 and Theorem 29 we discuss the convergence properties of the approximations. The proofs rely on the lower bound (32) for the tail of the sum of Grunwald weights (31).

The Grünwald weights \( w^{(\alpha)}_n \) are computed recursively as

\[
\begin{align*}
w^{(\alpha)}_0 &= 1, & w^{(\alpha)}_1 &= -\alpha, & w^{(\alpha)}_2 &= \frac{\alpha(\alpha - 1)}{2}, \\
w^{(\alpha)}_n &= (-1)^n \left( \frac{\alpha}{n} \right) = \left( 1 - \frac{\alpha + 1}{n} \right) w^{(\alpha)}_{n-1},
\end{align*}
\]

where \( \left\{ w^{(\alpha)}_n \right\}_{n=1}^{\infty} \) is an increasing sequence of negative numbers with sum

\[
\sum_{n=1}^{\infty} w^{(\alpha)}_n = -1. \tag{31}
\]

The Grünwald weights converge to zero with an asymptotic rate \[4\]

\[
|w^{(\alpha)}_n| \sim \frac{\alpha}{\Gamma(1-\alpha)} \frac{1}{n^{1+\alpha}} \quad \text{as} \ n \to \infty.
\]

We determine bounds for the Grünwald weights using the properties of the exponential function.

**Lemma 10. (Inequalities for the exponential function)**

(i) \( 1 - x < e^{-x} \) for \( 0 < x < 1 \);

(ii) \( 1 - x > e^{-x-x^2} \) for \( 0 < x < 2/3 \).

**Proof.** Let \( h(x) = e^{-x} + x - 1 \). The function \( h(x) \) has a positive derivative.

\[
h'(x) = 1 - e^{-x} > 1 - e^0 = 0.
\]

Therefore,

\[
h(x) = e^{-x} + x - 1 > h(0) = 0.
\]

Now we prove (ii). By taking logarithm from both sides

\[
\ln(1 - x) > -x - x^2.
\]
The function \( \ln(1 - x) \) has Maclaurin series

\[
\ln(1 - x) = -\sum_{n=1}^{\infty} \frac{x^n}{n} = -x - \frac{x^2}{2} - \sum_{n=3}^{\infty} \frac{x^n}{n}.
\]

Inequality (ii) is equivalent to

\[
\frac{x^2}{2} > \sum_{n=3}^{\infty} \frac{x^n}{n},
\]

\[
\frac{1}{2} > \frac{x}{3} + \frac{x^2}{4} + \frac{x^3}{5} + \sum_{n=6}^{\infty} \frac{x^{n-2}}{n}.
\]

We have that \(0 < x < 2/3\). Then

\[
\frac{x}{3} + \frac{x^2}{4} + \frac{x^3}{5} + \sum_{n=6}^{\infty} \frac{x^{n-2}}{n} < \frac{53}{135} + \frac{1}{6} \left( \frac{2}{3} \right)^4 \sum_{n=6}^{\infty} \frac{(2/3)^{n-6}}{n} < \frac{53}{135} + \frac{32}{2187} \sum_{n=6}^{\infty} \frac{(2/3)^{n-6}}{n},
\]

\[
\frac{x}{3} + \frac{x^2}{4} + \frac{x^3}{5} + \sum_{n=6}^{\infty} \frac{x^{n-2}}{n} < \frac{53}{135} + \frac{96}{2187} = \frac{1591}{3645} < \frac{1}{2}.
\]

In the next two lemmas we determine upper and lower bounds for \( |w_n^{(\alpha)}| \)
and \( \sum_{k=0}^{\infty} |w_k^{(\alpha)}| \).

**Lemma 11.** *(Estimates for Grünwald weights)*

\[ e^{-(\alpha+1)^2 \left( \frac{x^2}{2} - \frac{x}{2} \right)} \frac{\alpha(1-\alpha)2^\alpha}{n^{\alpha+1}} < |w_n^{(\alpha)}| < \frac{\alpha 2^{\alpha+1}}{(n+1)^{\alpha+1}}. \]

**Proof.** We determine bounds for the Grünwald weights from the recursive formula and the inequalities for the exponential function.

\[
|w_n^{(\alpha)}| = \left(1 - \frac{\alpha+1}{n}\right) |w_{n-1}^{(\alpha)}| < e^{-\frac{\alpha+1}{n}} |w_{n-1}^{(\alpha)}|,
\]

\[
|w_n^{(\alpha)}| < e^{-\frac{\alpha+1}{n}} |w_{n-1}^{(\alpha)}| < e^{-\frac{\alpha+1}{n}} e^{-\frac{\alpha+1}{n-1}} |w_{n-2}^{(\alpha)}|,
\]

\[
|w_n^{(\alpha)}| < e^{-\frac{\alpha+1}{n}} \cdots e^{-\frac{\alpha+1}{2}} |w_1^{(\alpha)}| = \alpha e^{-(\alpha+1) \sum_{k=2}^{n} \frac{1}{k}}.
\]

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The function $1/x$ is decreasing for $x \geq 0$. Then

$$\sum_{k=2}^{n} \frac{1}{k} > \int_{2}^{n+1} \frac{1}{x} \, dx = \ln(n + 1) - \ln 2$$

and

$$|w_n^{(\alpha)}| < \alpha e^{-(\alpha+1) \sum_{k=2}^{n} \frac{1}{k}} < \alpha e^{-(\alpha+1)(\ln(n+1)-\ln 2)} = \frac{\alpha^{\alpha+1}}{(n+1)^{\alpha+1}}.$$ 

Now we use the inequality for the exponential function from Lemma 10(ii) to determine a lower bound for the Grünwald weights.

$$|w_n^{(\alpha)}| = \left(1 - \frac{\alpha + 1}{n}\right)^{\left|w_n^{(\alpha)}\right|} > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} |w_n^{(\alpha)}|,$$

$$|w_n^{(\alpha)}| > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} \left|w_n^{(\alpha)}\right| > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} e^{-\frac{\alpha + 1}{n-1} - \left(\frac{\alpha + 1}{n-1}\right)^2} \left|w_n^{(\alpha)}\right|,$$

$$|w_n^{(\alpha)}| > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} e^{-\frac{\alpha + 1}{n-1} - \left(\frac{\alpha + 1}{n-1}\right)^2} \ldots e^{-\frac{\alpha + 1}{n-2} - \left(\frac{\alpha + 1}{n-2}\right)^2} \left|w_n^{(\alpha)}\right|,$$

$$|w_n^{(\alpha)}| > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} \frac{\alpha(1 - \alpha)}{2} e^{-(\alpha+1) \sum_{k=3}^{n} \frac{1}{k}} e^{-(\alpha+1)^2 \sum_{k=3}^{n} \frac{1}{k}},$$

$$|w_n^{(\alpha)}| > e^{-\frac{\alpha + 1}{n} - \left(\frac{\alpha + 1}{n}\right)^2} \frac{\alpha(1 - \alpha)}{2} e^{-(\alpha+1) \sum_{k=3}^{n} \frac{1}{k}} e^{-(\alpha+1)^2 \sum_{k=3}^{n} \frac{1}{k} \left(\frac{\pi^2}{6} - \frac{5}{4}\right)}.$$

We have that

$$\sum_{k=3}^{\infty} \frac{1}{k^2} = \sum_{k=1}^{\infty} \frac{1}{k^2} - 1 - \frac{1}{4} = \frac{\pi^2}{6} - \frac{5}{4}.$$ 

Then

$$|w_n^{(\alpha)}| > \frac{\alpha(1 - \alpha)}{2} e^{-(\alpha+1) \sum_{k=3}^{n} \frac{1}{k}} e^{-(\alpha+1)^2 \left(\frac{\pi^2}{6} - \frac{5}{4}\right)}.$$ 

The function $1/x$ is decreasing for $x \geq 0$. Then

$$\sum_{k=3}^{n} \frac{1}{k} < \int_{2}^{n} \frac{1}{x} \, dx = \ln n - \ln 2.$$ 

Hence,

$$|w_n^{(\alpha)}| > \frac{\alpha(1 - \alpha)}{2} e^{-(\alpha+1)^2 \left(\frac{\pi^2}{6} - \frac{5}{4}\right)} e^{-(\alpha+1)(\ln n - \ln 2)},$$

$$|w_n^{(\alpha)}| > e^{-(\alpha+1)^2 \left(\frac{\pi^2}{6} - \frac{5}{4}\right)} \frac{\alpha(1 - \alpha)2^\alpha}{n^{\alpha+1}}.$$

$\square$
We use the estimates for the Grünwald weights to determine bounds for the tail of (31).

**Lemma 12. (Bounds for sums of Grünwald weights)**

\[
\frac{1 - \alpha}{5} \left( \frac{2}{n} \right)^\alpha < \sum_{k=n}^\infty |w_k^{(\alpha)}| < 2 \left( \frac{2}{n} \right)^\alpha. \tag{32}
\]

**Proof.** From Lemma 11 we have

\[
\sum_{k=n}^\infty e^{-(\alpha+1)^2 \left( \frac{x^2}{\pi} - \frac{x}{4} \right) \frac{1 - \alpha}{n^{\alpha+1}}} < \sum_{k=n}^\infty |w_k^{(\alpha)}| < \sum_{k=n}^\infty \frac{\alpha^{2\alpha+1}}{(k+1)^{\alpha+1}}.
\]

The function \(1/x^{\alpha+1}\) is a decreasing for \(x \geq 0\) and we have:

\[
\sum_{k=n}^\infty \frac{1}{(k+1)^{\alpha+1}} < \frac{1}{\alpha n^\alpha} < \sum_{k=n}^\infty \frac{1}{k^{\alpha+1}}.
\]

Hence,

\[
e^{-(\alpha+1)^2 \left( \frac{x^2}{\pi} - \frac{x}{4} \right) \frac{1 - \alpha}{n^{\alpha}}} < \sum_{k=n}^\infty |w_k^{(\alpha)}| < \frac{2^{\alpha+1}}{n^\alpha}.
\]

The number \(\alpha\) is between zero and one. Then

\[
e^{-(\alpha+1)^2 \left( \frac{x^2}{\pi} - \frac{x}{4} \right)} > e^{-4 \left( \frac{x^2}{\pi} - \frac{x}{4} \right)} > \frac{1}{5}.
\]

\[\square\]

### 4.3 Third-order approximation

In the present section we use approximation (31) to determine recurrence relations for a third order approximation for equation (2), when the solution is sufficiently differentiable function. In section 4.2 we determined an estimate for sums of Grünwald weights. In Lemma 13 and Theorem 14 we use the lower bound to prove that the approximation converges to the solution with accuracy \(O(h^3)\), when the solution satisfies the conditions of Corollary 5.

\[
h^{-\alpha} \Delta_h^\alpha y_n = \left( \frac{a^2}{8} - \frac{5a}{24} \right) y_{n-2}^{(\alpha)} + \left( \frac{11a}{12} - \frac{a^2}{4} \right) y_{n-1}^{(\alpha)} + \left( 1 - \frac{17a}{4} + \frac{a^2}{8} \right) y_n^{(\alpha)} + O(h^3),
\]

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\[ \Delta_h^n y_n = h^\alpha \left( \frac{a^2}{8} - \frac{5a}{24} \right) (f_{n-2} - y_{n-2}) + h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) (f_{n-1} - y_{n-1}) + h^\alpha \left( 1 - \frac{17a}{4} + \frac{a^2}{8} \right) (f_n - y_n) + O \left( h^{3+\alpha} \right). \]

We have that
\[ \Delta_h^n y_n = \sum_{k=0}^{n} w_k^{(\alpha)} y_{n-k} = y_n + \sum_{k=1}^{n} w_k^{(\alpha)} y_{n-k}. \]

Let
\[ \gamma = 1 + h^\alpha \left( 1 - \frac{17a}{4} + \frac{a^2}{8} \right). \]

The solution of equation (2) satisfies
\[ y_n = \gamma^{-1} \left[ h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) (f_{n-1} - y_{n-1}) + h^\alpha \left( \frac{a^2}{8} - \frac{5a}{24} \right) (f_{n-2} - y_{n-2}) + h^\alpha \left( 1 - \frac{17a}{4} + \frac{a^2}{8} \right) f_n - \sum_{k=1}^{n} w_k^{(\alpha)} y_{n-k} \right] + O \left( h^{3+\alpha} \right). \]

We compute a numerical solution \( \tilde{y}_n \) with \( \tilde{y}_0 = \tilde{y}_1 = 0 \) and
\[ \tilde{y}_n = \gamma^{-1} \left[ h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) (f_{n-1} - \tilde{y}_{n-1}) + h^\alpha \left( \frac{a^2}{8} - \frac{5a}{24} \right) (f_{n-2} - \tilde{y}_{n-2}) + h^\alpha \left( 1 - \frac{17a}{4} + \frac{a^2}{8} \right) f_n - \sum_{k=1}^{n} w_k^{(\alpha)} \tilde{y}_{n-k} \right]. \quad (33) \]

Let \( e_n = y_n - \tilde{y}_n \) be the error of approximation (33). The numbers \( e_n \) satisfy
\[ e_n = -\gamma^{-1} \left[ h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) e_{n-1} + h^\alpha \left( \frac{a^2}{8} - \frac{5a}{24} \right) e_{n-2} + \sum_{k=1}^{n} w_k^{(\alpha)} e_{n-k} \right] + A_n, \]
where \( A_n \) is the truncation error of approximation (33). The numbers \( A_n \) satisfy
\[ |A_n| < Ah^{3+\alpha}, \]
where \( A \) is a constant such that
\[ A > \frac{(1-\alpha)2^\alpha D_{3+\alpha}}{10\Gamma(4+\alpha)}, \]
and
\[ D_{3+\alpha} = \max_{0 \leq x \leq 1} |y^{(3+\alpha)}(x)|. \]
We can represent the recurrence relations for the errors $e_n$ as
\[
e_n = \gamma^{-1} \left[ \left( \alpha - h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) \right) e_{n-1} + \left( \frac{\alpha(1 - \alpha)}{2} + h^\alpha \left( \frac{5a}{24} - \frac{a^2}{8} \right) \right) e_{n-2} - \sum_{k=3}^{n} w^{(\alpha)} e_{n-k} \right] + A_n,
\]
where
\[
\gamma_1 = \alpha - h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right), \quad \gamma_2 = \frac{\alpha(1 - \alpha)}{2} + h^\alpha \left( \frac{5a}{24} - \frac{a^2}{8} \right), \quad \gamma_k = -w^{(\alpha)}(k \geq 3).
\]

The numbers $\gamma_n$ are positive, because $h^\alpha < 1$ and $0 < \alpha < 1$.

**Lemma 13.** Suppose that equation (2) has sufficiently differentiable solution on the interval $[0, T]$ and $y(0) = y'(0) = y''(0) = y'''(0) = 0$. Then
\[
|e_n| < \left( \frac{10A}{(1 - \alpha)2^\alpha} \right) n^\alpha h^{3+\alpha}.
\]

**Proof.** We prove (35) by induction on $n$.

From the Generalized Mean Value Theorem
\[
e_1 = y_1 - \tilde{y}_1 = y(h) = \frac{y^{(3+\alpha)}(\xi)}{\Gamma(4 + \alpha)} h^{3+\alpha},
\]
\[
|e_1| < \frac{|y^{(3+\alpha)}(\xi)|}{\Gamma(4 + \alpha)} h^{3+\alpha} \leq \frac{D^{3+\alpha}}{\Gamma(4 + \alpha)} h^{3+\alpha} < \frac{10A}{(1 - \alpha)2^\alpha} h^{3+\alpha}.
\]

Suppose that (35) holds for all $n \leq \pi - 1$.

\[
|e_\pi| \leq \gamma^{-1} \left( \gamma_1|e_{\pi-1}| + \gamma_2|e_{\pi-2}| + \sum_{k=3}^{\pi-1} \gamma_k|e_{\pi-k}| \right) + |A_\pi|.
\]

By the induction hypothesis
\[
|e_{\pi-k}| < \frac{10A}{(1 - \alpha)2^\alpha} (\pi - k)\alpha h^{3+\alpha} < \frac{10}{(1 - \alpha)2^\alpha} \pi\alpha h^{3+\alpha} \quad (k = 1, \ldots, \pi - 1).
\]
Then
\[ |e_\pi| < \frac{10A\gamma^{-1}}{(1 - \alpha)2^\alpha} \pi^\alpha h^{3+\alpha} \sum_{k=1}^{\pi-1} \gamma_k + Ah^{3+\alpha}. \]  

(36)

We have that
\[ \sum_{k=1}^{\pi-1} \gamma_k = -h^\alpha \left( \frac{11a}{12} - \frac{a^2}{4} \right) + h^\alpha \left( \frac{5a}{24} - \frac{a^2}{8} \right) + \sum_{k=1}^{\pi-1} \left| w_k^{(\alpha)} \right|, \]
\[ \sum_{k=1}^{\pi-1} \gamma_k = h^\alpha \left( \frac{a^2}{8} - \frac{17a}{24} \right) + \sum_{k=1}^{\pi-1} \left| w_k^{(\alpha)} \right| - \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right|, \]
\[ \sum_{k=1}^{\pi-1} \gamma_k = 1 + h^\alpha \left( \frac{a^2}{8} - \frac{17a}{24} \right) - \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right| = \gamma - h^\alpha - \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right|. \]

Hence,
\[ \sum_{k=1}^{\pi-1} \left| \gamma_k \right| < \gamma - \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right|. \]  

(37)

From (36) and (37),
\[ |e_\pi| < \frac{10A\gamma^{-1}}{(1 - \alpha)2^\alpha} \pi^\alpha h^{3+\alpha} \left( \gamma - \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right| \right) + Ah^{3+\alpha}. \]

The number \( \gamma = 1 + h^\alpha \left( 1 - \frac{17a}{24} + \frac{a^2}{8} \right) \) satisfies
\[ 1 < \gamma < 2, \]
because \( h^\alpha < 1 \) and
\[ 1 - \frac{17a}{24} + \frac{a^2}{8} > 1 - \frac{17}{24} > \frac{7}{24} > 0, \]
\[ 1 - \frac{17a}{24} + \frac{a^2}{8} < 1 - \frac{17a}{24} + \frac{17a^2}{24} < 1. \]

Then
\[ \frac{1}{2} < \gamma^{-1} < 1 \]

and
\[ |e_\pi| \leq \frac{10A}{(1 - \alpha)2^\alpha} \pi^\alpha h^{3+\alpha} \left( 1 - \gamma^{-1} \sum_{k=\pi}^{\infty} \left| w_k^{(\alpha)} \right| \right) + Ah^{3+\alpha}, \]

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$$|e_n| < \frac{10A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha} - \frac{5A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha} \sum_{k=\pi}^{\infty} |w_k^{(\alpha)}| + Ah^{3+\alpha}.$$ 

In Lemma 12 we showed that
$$\sum_{k=\pi}^{\infty} |w_k^{(\alpha)}| > \frac{1-\alpha}{3} \left( \frac{2}{n} \right)^\alpha.$$ 

Hence,
$$|e_n| < \frac{10A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha} - \frac{5A}{(1-\alpha)2^\alpha} \frac{1-\alpha}{5} \left( \frac{2}{n} \right)^\alpha n^{\alpha} h^{3+\alpha} + Ah^{3+\alpha},$$
$$|e_n| < \frac{10A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha} - Ah^{3+\alpha} + Ah^{3+\alpha} = \frac{10A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha}.$$ 

In the next theorem we determine the order of approximation (33) on the interval $[0, T]$.

**Theorem 14.** Suppose that the solution of equation (2) satisfies
$$y(0) = y'(0) = y''(0) = y'''(0) = 0.$$ 

Then approximation (33) converges to the solution with accuracy $O(h^3)$.

**Proof.** The point $x_n = nh$ is in the interval $[0, T]$ when
$$n \leq N = \frac{T}{h}$$
because $T = Nh$. From Lemma 13
$$|e_n| < \frac{10A}{(1-\alpha)2^\alpha} n^{\alpha} h^{3+\alpha} \leq \frac{10A}{(1-\alpha)2^\alpha} \frac{T^\alpha}{h^\alpha} h^{3+\alpha},$$
$$|e_n| < \left( \frac{10AT^\alpha}{(1-\alpha)2^\alpha} \right) h^3.$$ 

**Lemma 15.** Suppose that equation (2) has a sufficiently smooth solution.

$$L_3 = \lim_{x \to 0} \left( \frac{d^2}{dx^2} f^{(1-\alpha)}(x) - \frac{L_1 x^{\alpha-2}}{\Gamma(\alpha)} - \frac{L_2 x^{\alpha-1}}{\Gamma(\alpha - 1)} \right).$$
Proof. By differentiating equation (2) we obtain

\[ y''(x) + y^{(1+(-1-\alpha))}(x) = f^{(1+(-1-\alpha))}(x), \]
\[ y'''(x) + y^{(2+(-1-\alpha))}(x) = f^{(2+(-1-\alpha))}(x). \]

From (28),

\[ y^{(2+(-1-\alpha))}(x) = \frac{d}{dx} y^{(1+(-1-\alpha))}(x) = \frac{d}{dx} \left( \frac{y'(0)x^{\alpha-1}}{\Gamma(\alpha)} + \frac{1}{\Gamma(\alpha)} \int_0^x \frac{y''(\xi)}{(x-\xi)^{1-\alpha}} d\xi \right). \]

Using integration by parts we obtain

\[ y^{(2+(-1-\alpha))}(x) = y'(0)x^{\alpha-2} + \frac{y''(0)x^{\alpha-1}}{\Gamma(\alpha)} + \frac{1}{\Gamma(\alpha)} \int_0^x \frac{y''(\xi)}{(x-\xi)^{1-\alpha}} d\xi, \]
\[ y^{(2+(-1-\alpha))}(x) = \frac{L_2x^{\alpha-1}}{\Gamma(\alpha)} + \frac{L_1x^{\alpha-2}}{\Gamma(\alpha-1)} + D_x^{3-\alpha} y(x). \]

Then

\[ y''(x) = f^{(2+(-1-\alpha))}(x) - \frac{L_2x^{\alpha-1}}{\Gamma(\alpha)} - \frac{L_1x^{\alpha-2}}{\Gamma(\alpha-1)} - D_x^{3-\alpha} y(x). \]

The value of \( D_x^{3-\alpha} y(0) \) is zero, when \( y(x) \) is sufficiently differentiable function.

\[ y'''(0) = \lim_{x \downarrow 0} \left( \frac{d^2}{dx^2} f^{(1-\alpha)}(x) - L_2x^{\alpha-1}/\Gamma(\alpha) - L_1x^{\alpha-2}/\Gamma(\alpha-1) \right). \]

Let

\[ z(x) = y(x) - L_1x - \frac{L_2}{2}x^2 - \frac{L_3}{6}x^3. \]

Lemma 16. The function \( z(x) \) satisfies

\[ z(0) = z'(0) = z''(0) = z'''(0) = 0 \]

and is a solution of the ordinary fractional differential equation

\[ z^{(\alpha)}(x) + z(x) = F(x), \quad (38) \]

where

\[ F(x) = f(x) - L_1x - \frac{L_2}{2}x^2 - \frac{L_3}{6}x^3 - \frac{L_1x^{1-\alpha}}{\Gamma(2-\alpha)} - \frac{L_2x^{2-\alpha}}{\Gamma(3-\alpha)} - \frac{L_3x^{3-\alpha}}{\Gamma(4-\alpha)}. \]

From Theorem 14 we can compute a third order numerical solution of equation (38) with recurrence relations (33).
4.4 Numerical examples

In Lemma 8, we showed that when equation (2) has a sufficiently differentiable solution the function \( f(x) \) satisfies the following conditions.

(C1) \( f(0) = 0; \)

(C2) The following limits exist

\[
\lim_{x \downarrow 0} f^{(1-\alpha)}(x) = L_1, \quad \lim_{x \downarrow 0} \left( \frac{d}{dx} f^{(1-\alpha)}(x) - \frac{L_1 x^{\alpha-1}}{\Gamma(\alpha)} \right) = L_2.
\]

When \( L_1 = L_2 = 0 \) the solution \( y(x) \) of (2) satisfies \( y'(0) = y''(0) = 0 \). The value of \( L_3 = y'''(0) \) is determined from the following limit.

\[
\lim_{x \downarrow 0} \left( \frac{d^2}{dx^2} f^{(1-\alpha)}(x) - \frac{L_1 x^{\alpha-2}}{\Gamma(\alpha)} - \frac{L_2 x^{\alpha-1}}{\Gamma(\alpha - 1)} \right) = L_3.
\]

In Example 1 we use the algorithms from Lemma 9 and Lemma 16 to compute second and third order numerical solutions for equation (2) with right-hand side (39). In Example 2 we consider equations (42) and (43) for which the conditions (C1) and (C2) are not satisfied.

4.4.1 Example 1

Consider the ordinary fractional differential equation

\[
\left\{ \begin{array}{l}
y^{(\alpha)}(x) + y(x) = f(x), \\
y(0) = 0.
\end{array} \right.
\]

with right-hand side

\[
f(x) = 2x + 3x^2 + 4x^3 + 6x^{3+\alpha} + \frac{2x^{1-\alpha}}{\Gamma(2 - \alpha)} + \frac{6x^{2-\alpha}}{\Gamma(3 - \alpha)} + \frac{24x^{3-\alpha}}{\Gamma(4 - \alpha)} + \Gamma(4 + \alpha)x^3.
\]

The function \( f(x) \) satisfies \( f(0) = 0 \),

\[
f^{(1-\alpha)}(x) = \frac{2x^\alpha}{\Gamma(1 + \alpha)} + \frac{6x^{1+\alpha}}{\Gamma(2 + \alpha)} + \frac{24x^{2+\alpha}}{\Gamma(3 + \alpha)} + \frac{\Gamma(4 + \alpha)x^{2+2\alpha}}{\Gamma(3 + 2\alpha)} + 2 + 6x + 12x^2 + 6(3 + \alpha)x^{2+\alpha}.
\]
Then $L_1 = f^{(1-\alpha)}(0) = 2$. Now we compute the value of $L_2 = y''(0)$.

$$\frac{d}{dx} f^{(1-\alpha)}(x) = \frac{2x^{\alpha - 1}}{\Gamma(\alpha)} + \frac{6x^\alpha}{\Gamma(1 + \alpha)} + \frac{24x^{\alpha + 1}}{\Gamma(2 + \alpha)} + \frac{\Gamma(4 + \alpha)x^{1 + 2\alpha}}{\Gamma(2 + 2\alpha)} + 6 + 24x + 6(2 + \alpha)(3 + \alpha)x^{1 + \alpha}$$

$$L_2 = \lim_{x \to 0} \left( \frac{d}{dx} f^{(1-\alpha)}(x) - \frac{2x^{\alpha - 1}}{\Gamma(\alpha)} \right) = 6.$$ Let

$$F_1(x) = f(x) - L_1 x - \frac{L_2}{2} x^2 - \frac{L_1}{\Gamma(2 - \alpha)} x^{1 - \alpha} - \frac{L_2}{\Gamma(3 - \alpha)} x^{2 - \alpha},$$

$$F_1(x) = 4x^3 + 6x^{3+\alpha} + \frac{24x^{3-\alpha}}{\Gamma(4 - \alpha)} + \Gamma(4 + \alpha)x^3.$$ The function $z_1(x) = y(x) - 2x - 3x^2$ is a solution of

$$z_1^{(\alpha)}(x) + z_1(x) = 4x^3 + 6x^{3+\alpha} + \frac{24x^{3-\alpha}}{\Gamma(4 - \alpha)} + \Gamma(4 + \alpha)x^3. \quad (40)$$

The solution of equation (40) is $z_1(x) = 4x^3 + 6x^{3+\alpha}$. From Theorem 7, we can compute second order numerical solutions of equation (40) with approximations (25) and (26). Experimental results for approximation (26) and $\alpha = 0.25$ are given in Table 3 and Figure 2.

$$\frac{d^2}{dx^2} f^{(1-\alpha)}(x) = \frac{2x^{\alpha - 1}}{\Gamma(\alpha - 2)} + \frac{6x^\alpha}{\Gamma(1 + \alpha)} + \frac{24x^\alpha}{\Gamma(1 + 2\alpha)} + \frac{\Gamma(4 + \alpha)x^{2\alpha}}{\Gamma(2 + 2\alpha)} + 24 + 6(\alpha + 1)(\alpha + 2)(\alpha + 3)x^{\alpha},$$

$$L_3 = \lim_{x \to 0} \left( \frac{d^2}{dx^2} f^{(1-\alpha)}(x) - \frac{2x^{\alpha - 2}}{\Gamma(\alpha)} - \frac{6x^{\alpha - 1}}{\Gamma(\alpha - 1)} \right) = 24.$$ Let

$$F_2(x) = f(x) - L_0 - L_1 x - \frac{L_2}{2} x^2 - \frac{L_3}{6} x^3 - \frac{L_1 x^{1-\alpha}}{\Gamma(2 - \alpha)} - \frac{L_2 x^{2-\alpha}}{\Gamma(3 - \alpha)} - \frac{L_3 x^{3-\alpha}}{\Gamma(4 - \alpha)},$$

$$F_2(x) = 6x^{3+\alpha} + \Gamma(4 + \alpha)x^3.$$ The function $z_2(x) = y(x) - 1 - 2x - 3x^2 - 4x^3$ is a solution of the equation

$$z_2^{(\alpha)}(x) + z_2(x) = 6x^{3+\alpha} + \Gamma(4 + \alpha)x^3. \quad (41)$$

Equation (41) has solution $z_2(x) = 6x^{3+\alpha}$. Experimental results for a third order numerical solution of equation (41) using recurrence relations (33) are given in Table 4 and Figure 3.
Figure 2: Graph of the solution of equation (40) and second order approximation (26) for $h = 0.05$ and $\alpha = 0.25$.

Figure 3: Graph of the solution of equation (41) and third order approximation (33) for $h = 0.05$ and $\alpha = 0.75$.

Table 3: Maximum error and order of approximation (26) for equation (40) with $\alpha = 1/4$.

| $h$   | Error     | Ratio     | Order     |
|-------|-----------|-----------|-----------|
| 0.05  | 0.00393827| 3.93462   | 1.97622   |
| 0.025 | 0.00099263| 3.96753   | 1.98824   |
| 0.0125| 0.00024916| 3.98382   | 1.99415   |
| 0.00625| 0.00006242| 3.99192   | 1.99708   |
| 0.003125| 0.00001562| 3.99596   | 1.99854   |

Table 4: Maximum error and order of approximation (33) for equation (41) with $\alpha = 3/4$.

| $h$    | Error     | Ratio     | Order     |
|--------|-----------|-----------|-----------|
| 0.05   | 0.000314897| 7.52526   | 2.91174   |
| 0.025  | 0.000040446| 7.78566   | 2.96082   |
| 0.0125 | $5.121 \times 10^{-6}$ | 7.89840   | 2.98156   |
| 0.00625| $6.441 \times 10^{-7}$ | 7.95061   | 2.99107   |
| 0.003125| $8.075 \times 10^{-8}$ | 7.97568   | 2.99561   |
Table 5: Maximum error and order of approximation (25) for equation (42).

| $h$   | Error      | Ratio      | $\log_2(Ratio)$ |
|-------|------------|------------|-----------------|
| 0.0125| 0.0162401  | 1.03445    | 0.048863        |
| 0.00625| 0.0152728 | 1.06333    | 0.088589        |
| 0.003125| 0.0140672 | 1.08571    | 0.118636        |
| 0.0015625| 0.0127479 | 1.10349    | 0.142075        |
| 0.00078125| 0.0114037 | 1.11787    | 0.160754        |

4.4.2 Example 2

We compute numerical solutions for two ordinary fractional differential equations for which the conditions (C1) and (C2) for differentiable solution are not satisfied.

$$y^{(0.25)}(x) + y(x) = x^{0.25} + \Gamma(1.25).$$  \hspace{1cm} (42)

The solution of equation (42) is $y(x) = x^{0.25}$. The solution is not a continuously differentiable function, because condition (C1) is not satisfied

$$f(0) = \Gamma(1.25) \neq 0.$$  \hspace{1cm} (42)

We compute a numerical solution of equation (42) with recurrence relations (25). When $h = 0.025$ the error is 0.0167995. The approximation converges to the solution with a very slow rate and the approximation order is smaller than one. Experimental results are given in Table 5.

The following equation has solution $y(x) = x^{1.25}$.

$$y^{(0.25)}(x) + y(x) = \Gamma(1.25)x + x^{1.25}.$$  \hspace{1cm} (43)

The solution is equation (43) has better differentiability properties than the solution of equation (42). We can expect that approximation (25) has higher accuracy for equation (43).

$$f(x) = \Gamma(1.25)x + x^{1.25}, \quad (f(0) = 0).$$

$$f^{(0.75)}(x) = x^{0.25} + \frac{\Gamma(2.25)}{\Gamma(1.5)}x^{0.5}, \quad L_1 = \lim_{x \to 0} f^{(0.75)}(x) = 0.$$  \hspace{1cm} (43)

$$\frac{d}{dx}f^{(0.75)}(x) = \frac{0.25}{x^{0.5}} + \frac{\Gamma(2.25)}{\Gamma(0.5)x^{0.5}}, \quad L_2 = \lim_{x \to 0} \frac{d}{dx}f^{(0.75)}(x) = \infty.$$  \hspace{1cm} (43)

The solution of equation (43) doesn’t have a continuous second derivative on the interval $[0, 1]$, because condition (C2) is not satisfied. When $h = 0.025$ the error is 0.000148. The accuracy of approximation (25) for equation (43) is around $O(h^{1.31})$, when $h > 0.0008$ (Table 6).
Table 6: Maximum error and order of approximation \((25)\) for equation \((42)\).

| \(h\)     | Error       | Ratio   | Order    |
|-----------|-------------|---------|----------|
| \(0.0125\) | 0.0000589415 | 2.50814 | 1.32662  |
| \(0.00625\) | 0.0000235523 | 2.50259 | 1.32342  |
| \(0.003125\) | 9.4369 \times 10^{-6} | 2.49576 | 1.31948  |
| \(0.0015625\) | 3.7930 \times 10^{-6} | 2.48797 | 1.31497  |
| \(0.00078125\) | 1.5297 \times 10^{-6} | 2.47954 | 1.31007  |

5 Second-order implicit difference approximations for the time fractional sub-diffusion equation

In the present section we determine implicit difference approximations for the fractional sub-diffusion equation. We show that when the solution of the sub-diffusion equation is a sufficiently differentiable function the difference approximations have second order accuracy \(O(\tau^2 + h^2)\). The analytic solution of the fractional sub-diffusion equation can be determined using Laplace-Fourier transform \([2]\) or separation of variables for special cases of the boundary conditions and the function \(G(x, t)\). The fractional diffusion equation

\[
\begin{cases} 
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2}, \\
 u(0, t) = u(1, t) = 0, u(x, 0) = g(x).
\end{cases}
\]  

(44)

has an analytical solution \([26]\).

\[
u(x, t) = 2 \sum_{n=1}^{\infty} c_n E_\alpha(-n^2 \pi^2 \tau^\alpha) \sin(n\pi x)
\]  

(45)

on the domain \(\{0 \leq x \leq 1, t \geq 0\}\), where

\[
c_n = \int_0^1 g(\xi) \sin(n\pi \xi) d\xi
\]

and \(E_\alpha\) is the one-parameter Mittag-Leffler function. Each term

\[E_\alpha(-n^2 \pi^2 \tau^\alpha) \sin(n\pi x)\]

is a solution of \((11)\) and its coefficient \(c_n\) is the coefficient of the Fourier sine series of the function \(g(x)\). The graph of the analytical solution of \((44)\) when \(g(x) = x^2(x - 1)\) is given in Figure 4.
Figure 4: Analytical solution of (44) for $\alpha = 1/2$, $g(x) = x^2(x - 1)$ and $0 \leq t \leq 0.05$.

5.1 Second order implicit difference approximation

The fractional sub-diffusion equation is an important equation in fractional calculus. The implicit difference approximation which uses approximation (6) for the fractional derivative and central difference approximation for the second derivative with respect to $x$, has accuracy $O(\tau^{2-\alpha} + h^2)$ [41]. Finite difference approximations are convenient way to approximate the solution of partial fractional differential equations. They combine simple description with stability and high accuracy. Even when the exact solution of the time-fractional diffusion equation is available, the finite difference approximations may have higher accuracy than approximations using the exact solution. The approximation error of a numerical solution of (44) computed by truncating (45) includes errors from the truncation of the Fourier series at the endpoints and the approximations of the coefficients $c_n$ and the Mittag-Leffler functions. In this section we determine second order difference approximations for equation (1) on the domain

$$D = [0, 1] \times [0, T].$$

We can assume that equation (1) has homogeneous initial and boundary conditions

$$\left\{ \begin{array}{l}
\frac{\partial^{\alpha} u(x, t)}{\partial t^{\alpha}} = \frac{\partial^2 u(x, t)}{\partial x^2} + G(x, t), \\
u(0, t) = u(1, t) = 0, u(x, 0) = 0.
\end{array} \right. \quad (46)$$
If equation (1) is given with non-homogeneous initial or boundary conditions the substitute
\[
\varphi(x, t) = u(x, t) - u(x, 0) - (1 - x)(u(0, t) - u(0, 0)) - x(u(1, t) - u(1, 0))
\]
converts the equation to equation which has the same form and homogeneous initial and boundary conditions. In Lemma 6, we showed that when the solution \( u(x, t) \) is sufficiently differentiable function with respect to the time variable \( t \), the fractional derivative \( \frac{\partial^\alpha u(x, 0)}{\partial t^\alpha} \) is zero when \( t = 0 \). When the solution \( u(x, t) \) has continuous second derivative \( u_{xx}(x, t) \) with respect to \( t \), the function \( G(x, t) \) satisfies the condition
\[
G(x, 0) = \left. \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} \right|_{t=0} - \left. \frac{\partial^2 u(x, t)}{\partial x^2} \right|_{t=0} = 0.
\]
This compatibility condition corresponds to the condition \( f(0) = 0 \) for differentiable solution of ordinary fractional differential equation (2), with initial condition \( y(0) = 0 \). In order to construct second order difference approximations for equation (44) using approximations (9) and (10) for the Caputo derivative, the first step is to ensure that the first and second derivatives of the solution \( u_t(x, t) \) and \( u_{tt}(x, t) \) with respect to the time variable \( t \) are equal to zero when \( t = 0 \). Let
\[
L_1(x) = \left. \frac{\partial u(x, t)}{\partial t} \right|_{t=0}, \quad L_2(x) = \left. \frac{\partial^2 u(x, 0)}{\partial t^2} \right|_{t=0}, \quad L(x) = \left. \frac{\partial^3 u(x, 0)}{\partial t \partial x^2} \right|_{t=0}.
\]
By applying time fractional derivative of order \( 1 - \alpha \) to equation (1) we obtain
\[
\frac{\partial u(x, t)}{\partial t} = \frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} + \frac{\partial^{1-\alpha} G(x, t)}{t^{1-\alpha}}.
\]
When \( u_{xx}(x, t) \) is bounded in \( D \), we have that \( \frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} = 0 \). Then
\[
L_1(x) = \left. \frac{\partial^{1-\alpha} G(x, t)}{t^{1-\alpha}} \right|_{t=0} = 0.
\]
By differentiating (47) with respect to \( t \) we obtain
\[
\frac{\partial^2 u(x, t)}{\partial t^2} = \frac{\partial}{\partial t} \frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} G(x, t)}{t^{1-\alpha}}.
\]
The Caputo derivative of order \( 1 - \alpha \) of the function \( u_{xx}(x, t) \) with respect to \( t \) is defined as
\[
\frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} = \frac{1}{\Gamma(\alpha)} \int_0^t \frac{\partial^3 u(x, \xi)}{\partial t \partial x^2} (t - \xi)^{\alpha-1} d\xi.
\]
After integration by parts and differentiation with respect to \( t \) we obtain
\[
\frac{\partial}{\partial t} \frac{\partial^{3-\alpha} u(x,t)}{\partial t^{1-\alpha} \partial x^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \frac{\partial^3 u(x,t)}{\partial t^3 \partial x^2} \bigg|_{t=0} + \frac{1}{\Gamma(\alpha)} \int_0^t \frac{\partial^4 u(x,\xi)}{\partial t^2 \partial x^2}(t-\xi)^{\alpha-1}d\xi.
\]
From the definition of Caputo derivative of order \( 2 - \alpha \) with respect to \( t \)
\[
\frac{1}{\Gamma(\alpha)} \int_0^t \frac{\partial^4 u(x,\xi)}{\partial t^2 \partial x^2}(t-\xi)^{\alpha-1}d\xi = D_t^{2-\alpha} \frac{\partial^2 u(x,t)}{\partial x^2}.
\]
So,
\[
\frac{\partial}{\partial t} \frac{\partial^{3-\alpha} u(x,t)}{\partial t^{1-\alpha} \partial x^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} L(x) + D_t^{2-\alpha} \frac{\partial^2 u(x,t)}{\partial x^2}.
\]
(50)
We have that
\[
\frac{\partial^3 u(x,t)}{\partial t \partial x^2} = \frac{\partial}{\partial t} \left( \frac{\partial^3 u(x,t)}{\partial t^2} - G(x,t) \right) = \frac{\partial}{\partial t} \frac{\partial^3 u(x,t)}{\partial t^2} - \frac{\partial}{\partial t} G(x,t).
\]
By integrating by parts and differentiating with respect to \( t \)
\[
\frac{\partial}{\partial t} \frac{\partial^3 u(x,t)}{\partial t^2} = \frac{\partial u(x,0)}{\partial t} \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial^2 u(x,\xi)}{\partial t^2}(t-\xi)^{\alpha}d\xi - \frac{\partial}{\partial t} G(x,t).
\]
Then
\[
\frac{\partial^3 u(x,t)}{\partial t \partial x^2} = \frac{\partial u(x,0)}{\partial t} \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial^2 u(x,\xi)}{\partial t^2}(t-\xi)^{\alpha}d\xi - \frac{\partial}{\partial t} G(x,t),
\]
\[
\frac{\partial^3 u(x,t)}{\partial t \partial x^2} = \frac{L_1(x)}{\Gamma(1-\alpha)t^\alpha} + D_t^{1+\alpha} u(x,t) - \frac{\partial}{\partial t} G(x,t).
\]
The function \( L(x) \) is computed as
\[
L(x) = \left. \frac{\partial^3 u(x,t)}{\partial t \partial x^2} \right|_{t=0} = \lim_{t \downarrow 0} \left( \frac{L_1(x)}{\Gamma(1-\alpha)t^\alpha} - \frac{\partial}{\partial t} G(x,t) \right)
\]
(51)
because the Caputo derivative \( D_t^{1+\alpha} u(x,0) \) is zero when \( u_t(x,t) \) is bounded.
The function \( L_2(x) \) is computed from (49) and (50)
\[
\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} L(x) + D_t^{2-\alpha} \frac{\partial^2 u(x,t)}{\partial x^2} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} G(x,t)}{t^{1-\alpha}},
\]
\[
L_2(x) = \frac{\partial^2 u(x,0)}{\partial t^2} = \lim_{t \downarrow 0} \left( \frac{L(x)}{\Gamma(\alpha)t^{1-\alpha}} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} G(x,t)}{t^{1-\alpha}} \right).
\]
(52)
Let
\[ v(x, t) = u(x, t) - L_1(x)t - \frac{L_2(x)}{2}t^2. \]
The partial derivatives \( v_t(x, t) \) and \( v_{tt}(x, t) \) of the function \( v(x, t) \) are equal to zero when \( t = 0 \).
\[
\frac{\partial^\alpha v(x, t)}{\partial t^\alpha} = \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} - \frac{L_1(x)t^{1-\alpha}}{\Gamma(2 - \alpha)} - \frac{L_2(x)t^{2-\alpha}}{\Gamma(3 - \alpha)},
\]
\[
\frac{\partial^2 v(x, t)}{\partial x^2} = \frac{\partial^2 u(x, t)}{\partial x^2} - L'_1(x)t - \frac{L''_2(x)}{2}t^2.
\]
The function \( v(x, t) \) is solution of the fractional sub-diffusion equation
\[
\begin{cases}
\frac{\partial^\alpha v(x, t)}{\partial t^\alpha} = \frac{\partial^2 v(x, t)}{\partial x^2} + H(x, t), \\
v(0, t) = v(1, t) = 0, v(x, 0) = 0,
\end{cases}
\]
where
\[
H(x, t) = G(x, t) - \frac{L_1(x)t^{1-\alpha}}{\Gamma(2 - \alpha)} - \frac{L_2(x)t^{2-\alpha}}{\Gamma(3 - \alpha)} + L'_1(x)t + \frac{L''_2(x)}{2}t^2.
\]
In section 4 we used approximation (10) to determine second order numerical solutions [25] and [26] for equation (2). Now we use (10) and a central difference approximation for \( u_{xx}(x, t) \) to construct implicit difference approximations (56) and (57) for equation (53). In Theorem 29 we show that the difference approximations are unconditionally stable and have second order accuracy \( O(\tau^2 + h^2) \). Let \( h = 1/N \) and \( \tau = T/M \) where \( M \) and \( N \) are positive integers, and
\[ x_n = nh, \quad t_m = m\tau, \quad v_n^m = v(x_n, t_m), \quad H_n^m = H(x_n, t_m). \]
From approximation (10) and equation (53)
\[
\Delta_h^\alpha v(x_n, t_m) = \left( \frac{\alpha}{2} \right) \frac{\partial^\alpha v(x_n, t_{m-1})}{\partial t^\alpha} + \left( 1 - \frac{\alpha}{2} \right) \frac{\partial^2 v(x_n, t_m)}{\partial x^2} + O(\tau^2)
\]
\[
= \left( \frac{\alpha}{2} \right) \frac{\partial^2 v(x_n, t_{m-1})}{\partial x^2} + \left( 1 - \frac{\alpha}{2} \right) \frac{\partial^2 v(x_n, t_m)}{\partial x^2} + \left( \frac{\alpha}{2} \right) H_n^{m-1} + \left( 1 - \frac{\alpha}{2} \right) H_n^m + O(\tau^2).
\]
By approximating the second derivatives \( u_{xx}(x_n, t_{m-1}) \) and \( u_{xx}(x_n, t_m) \) with central difference formulas we obtain
\[
\frac{1}{\tau^\alpha} \sum_{k=0}^{m} w_k^{(\alpha)} v_n^{m-k} + O(\tau^2 + h^2) = \left( 1 - \frac{\alpha}{2} \right) \frac{v_{n+1}^{m} - 2v_n^m + v_{n-1}^m}{h^2}
\]
\[
+ \left( \frac{\alpha}{2} \right) v_{n+1}^{m} - 2v_n^m + v_{n-1}^m + \left( \frac{\alpha}{2} \right) H_n^{m-1} + \left( 1 - \frac{\alpha}{2} \right) H_n^m.
\]
Let \( \eta = \frac{\alpha}{h^2}. \) The solution of equation (53) satisfies

\[
v_m^n - \left(1 - \frac{\alpha}{2}\right) \eta (v_{n-1}^m - 2v_n^m + v_{n+1}^m) + \tau^\alpha O \left(\tau^2 + h^2\right) = -\sum_{k=2}^{m} w_k^{(\alpha)} m^{m-k}
\]

\[
+ \alpha v_n^{m-1} + \frac{\alpha \eta}{2} (v_{n-1}^m - 2v_n^m + v_{n+1}^m) + \tau^\alpha \left(\left(\frac{\alpha}{2}\right) H_{n-1}^m + \left(1 - \frac{\alpha}{2}\right) \frac{H_n}{n-1}\right).
\]

Let \( x = (x_n) \) be an \( N - 1 \) dimensional vector. The maximum (infinity) norm of the vector \( x \) is

\[
\|x\| = \max_{1 \leq n \leq N - 1} |x_n|.
\]

Define the vectors \( V_m, H_m \) and \( K_m \) as

- \( V_m = (v_n^m)_{n=1}^{N-1} \) - a vector of values of the exact solution at time \( t = m\tau; \)
- \( H_m = \left(\left(\frac{\alpha}{2}\right) H_{n-1}^m + \left(1 - \frac{\alpha}{2}\right) \frac{H_n}{n-1}\right)_{n=1}^{N-1}; \)
- \( K_m = (k_n^m)_{n=1}^{N-1} \) - a vector of the truncation errors at \( t = m\tau. \) In (55) we showed that \( \|K_m\| \in O \left(\tau^\alpha \left(\tau^2 + h^2\right)\right). \) The elements of the vector \( K_m \) satisfy

\[
|k_n^m| < K \tau^\alpha \left(\tau^2 + h^2\right),
\]

where \( K > 1 \) is a positive constant (The conditions \( K > 1 \) and (62) guarantee that \( C_R > 1 \)).

Let \( g_n^{(\alpha)} = -w_n^{(\alpha)} \) and \( A = A_{N-1} \) be a tridiagonal square matrix with entries 2 on the main diagonal and \(-1\) on the first diagonals below and above the main diagonal.

\[
A_5 = \begin{pmatrix}
2 & -1 & 0 & 0 & 0 \\
-1 & 2 & -1 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 \\
0 & 0 & -1 & 2 & -1 \\
0 & 0 & 0 & -1 & 2
\end{pmatrix}, \quad X_5 = \begin{pmatrix}
b & a & 0 & 0 & 0 \\
c & b & a & 0 & 0 \\
0 & c & b & a & 0 \\
0 & 0 & c & b & a \\
0 & 0 & 0 & c & b
\end{pmatrix}.
\]

The numbers \( g_n^{(\alpha)} \) are positive for \( n \geq 1 \) and \( \sum_{n=1}^{\infty} g_n^{(\alpha)} = 1. \) The eigenvalues of the matrix \( A \) are determined from the following more general result for eigenvalues of a tridiagonal matrix [24].

**Lemma 17.** The eigenvalues of the tridiagonal matrix \( X = X_{N-1} \) with entries \( b \) on the main diagonal and \( a \) and \( c \) on the first diagonals above and below the main diagonal are given by

\[
\lambda_k = b + 2a \sqrt{\frac{c}{a} \cos \left(\frac{k\pi}{N}\right)}, \quad (k = 1, 2, \ldots, N - 1).
\]
Corollary 18. The matrix $A$ has eigenvalues

$$\lambda_k = 4 \sin^2 \left( \frac{k \pi}{N} \right), \quad (k = 1, \cdots, N - 1).$$

Proof. From Lemma 5 with $a = c = -1$ and $b = 2$ we obtain

$$\lambda_k = 2 - 2 \cos \left( \frac{k \pi}{N} \right) = 4 \sin^2 \left( \frac{k \pi}{N} \right).$$

Equation (55) is written in a matrix form as

\[
\left( I + \left(1 - \frac{\alpha}{2}\right) \eta A \right) V_m = \left(\alpha I - \frac{\alpha \eta}{2} A\right) V_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} V_{m-k} + \tau^\alpha H_m + K_m.
\]

Let $P$ and $Q$ be the following matrices.

$$P = I + \left(1 - \frac{\alpha}{2}\right) \eta A, \quad Q = I - \frac{\eta}{2} A.$$

Then

$$PV_m = \alpha QV_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} V_{m-k} + \tau^\alpha H_m + K_m.$$

We compute an approximation $\tilde{V}_m$ to the exact solution $V_m$ of equation (53) at time $t_m = m \tau$ on the grid

\[
\{(x_n, t_m) | 1 \leq n \leq N, 1 \leq m \leq M \}
\]

with $\tilde{V}_0 = 0$ and the linear systems

\[
P\tilde{V}_m = \alpha Q\tilde{V}_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} \tilde{V}_{m-k} + \tau^\alpha H_m.
\] (56)

The values of the elements of the vector $H_m$ satisfy

\[
\left(\frac{\alpha}{2}\right) H_{n}^{m-1} + \left(1 - \frac{\alpha}{2}\right) H_{n}^{m} = H_{n}^{m-\alpha/2} + O(\tau^2).
\]

Another difference approximation for equation (53) is computed recursively with the linear systems

\[
P\tilde{V}_m = \alpha Q\tilde{V}_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} \tilde{V}_{m-k} + \tau^\alpha H_m.
\] (57)
where \( H_m = \left( H_n^{m-\alpha/2} \right)^{N-1} \). In Theorem 29 we show that the implicit difference approximations (56) and (57) are unconditionally stable and have second order accuracy with respect to the space and time variables. The proof relies on the positivity of the eigenvalues of the matrix \( A \) and the lower bound (32) for sums of Grünwald weights.

5.2 Numerical example

We compute numerical solutions of the fractional sub-diffusion equation (1) with homogeneous initial and boundary conditions. The difference approximations (56) and (57) have comparable properties. In some experiments the truncation error of (57) is smaller than the truncation error of (56), and it has slightly better overall performance. When

\[
G(x, t) = \frac{a(x)t^{1-\alpha}}{\Gamma(2 - \alpha)} + \frac{2b(x)t^{2-\alpha}}{\Gamma(3 - \alpha)} + \frac{\Gamma(3 + \alpha)c(x)t^2}{2} - a''(x)t - b''(x)t^2 - c''(x)t^{2+\alpha}
\]

equation (46) has solution

\[
u(x, t) = a(x)t + b(x)t^2 + c(x)t^{2+\alpha}.
\]

The first step is to compute the functions \( L_1(x), L(x) \) and \( L_2(x) \).

\[
L_1(x) = \left. \frac{\partial^{1-\alpha}G(x, t)}{t^{1-\alpha}} \right|_{t=0}, \quad L(x) = \lim_{t\downarrow 0} \left( \frac{L_1(x)}{1 - \alpha} \frac{\partial}{\partial t} G(x, t) \right),
\]

\[
L_2(x) = \lim_{t\downarrow 0} \left( \frac{L(x)}{\Gamma(1-\alpha)t^{1-\alpha}} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha}G(x, t)}{t^{1-\alpha}} \right),
\]

\[
\frac{\partial^{1-\alpha}G(x, t)}{\partial t^{1-\alpha}} = a(x) + 2b(x)t + (2+\alpha)c(x)t^{1+\alpha} - \frac{a''(x)t^\alpha}{\Gamma(1 + \alpha)} - \frac{2b''(x)t^{1+\alpha}}{\Gamma(2 + \alpha)} - \frac{\Gamma(3 + \alpha)c''(x)t^{2+\alpha}}{\Gamma(2 + 2\alpha)}.
\]

By setting \( t = 0 \) we obtain

\[
L_1(x) = a(x),
\]

\[
\frac{\partial}{\partial t} G(x, t) = \frac{a(x)t^{-\alpha}}{\Gamma(1 - \alpha)} + \frac{2b(x)t^{1-\alpha}}{\Gamma(2 - \alpha)} + \Gamma(3+\alpha)c(x)t - a''(x)t - 2b''(x)t - (2+\alpha)c''(x)t^{1+\alpha},
\]

\[
L(x) = \lim_{t\downarrow 0} \left( \frac{a(x)}{\Gamma(1-\alpha)t^\alpha} - \frac{\partial}{\partial t} G(x, t) \right) = a''(x),
\]

\[
\frac{\partial}{\partial t} \frac{\partial^{1-\alpha}G(x, t)}{\partial t^{1-\alpha}} = 2b(x) + (1+\alpha)(2+\alpha)c(x)t^\alpha - \frac{a''(x)t^\alpha}{\Gamma(1 + \alpha)} - \frac{2b''(x)t^{\alpha}}{\Gamma(2 + \alpha)} - \frac{\Gamma(3 + \alpha)c''(x)t^{2\alpha}}{\Gamma(1 + 2\alpha)},
\]

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Figure 5: Graphs of the solution of equation (58) and approximation (57) for \( \alpha = 1/2 \) and \( h = \tau = 0.05 \) (left) and \( h = 0.025, \tau = 0.0125 \) at time \( t = 1 \).

Equation (58) has solution 

\[
L_2(x) = \lim_{t \to 0} \left( \frac{a''(x)}{\Gamma(\alpha)t^{1-\alpha}} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha}G(x,t)}{t^{1-\alpha}} \right) = 2b(x).
\]

Let

\[
v(x,t) = u(x,t) - L_1(x)t - \frac{L_2(x)}{2}t^2 = u(x,t) - a(x)t - b(x)t^2.
\]

The function \( v(x,t) \) is a solution of (53), where the function \( H(x,t) \) is computed from \( G(x,t) \) and the functions \( L_1(x) \) and \( L_2(x) \) with (54)

\[
H(x,t) = \frac{1}{2} \Gamma(3 + \alpha)c(x)t^2 - c''(x)t^{2+\alpha}
\]

the fractional sub-diffusion equation (53) has solution

\[
v(x,t) = c(x)t^{2+\alpha}.
\]

When \( c(x) = 2x^2(1-x) \) we obtain the following fractional diffusion equation

\[
\begin{cases}
\frac{\partial^\alpha v(x,t)}{\partial t^\alpha} = \frac{\partial^2 v(x,t)}{\partial x^2} + \Gamma(3 + \alpha)(1-x)x^2t^2 - 4(3x-1)t^{2+\alpha}, \\
v(0,t) = v(1,t) = 0, v(x,0) = 0.
\end{cases}
\tag{58}
\]

When \( h = \tau = 0.1 \) the error of difference approximation (57) for equation (58) at time \( t = 1 \) is 0.00097075. When \( h = 0.1 & \tau = 0.05 \) the error is 0.000243735. Experimental results for the maximum error and order of approximation (57) at time \( t = 1 \) are given in Figure 5, Table 7 and Table 8.
Table 7: Maximum error and order of approximation \([57]\) for equation \([58]\) with \(\alpha = 1/2\) and \(h = \tau\) at time \(t = 1\).

| \(h\)  | \(\tau\) | Error       | Ratio  | Order   |
|--------|--------|-------------|--------|---------|
| 0.05   | 0.05   | 0.000244392 | 3.97210| 1.98990 |
| 0.025  | 0.025  | 0.000061436 | 3.97802| 1.99205 |
| 0.0125 | 0.0125 | 0.000015376 | 3.99552| 1.99383 |
| 0.00625| 0.00625| 3.846 \times 10^{-6} | 3.99778| 1.99920 |
| 0.003125| 0.003125| 9.619 \times 10^{-7} | 3.99865| 1.99951 |

Table 8: Maximum error and order of approximation \([57]\) for equation \([58]\) with \(\alpha = 1/2\) and \(h = 2\tau\) at time \(t = 1\).

| \(h\)  | \(\tau\) | Error       | Ratio  | Order   |
|--------|--------|-------------|--------|---------|
| 0.05   | 0.025  | 0.000061232 | 3.98055| 1.99297 |
| 0.025  | 0.0125 | 0.000015376 | 3.98235| 1.99362 |
| 0.0125 | 0.00625| 3.846 \times 10^{-6} | 3.99770| 1.99917 |
| 0.00625| 0.003125| 9.618 \times 10^{-7} | 3.99888| 1.99959 |
| 0.003125| 0.0015625| 2.405 \times 10^{-7} | 3.99920| 1.99971 |

5.3 Numerical Analysis

Let \(E_m = V_m - \tilde{V}_m\) be the error vectors for difference approximations \([56]\) or \([57]\) at time \(t_m = m\tau\). The vectors \(E_m\) are computed recursively with \(E_0 = 0\) and

\[
P E_m = \alpha Q E_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} E_{m-k} + K_m,
\]

where

\[
P = I + \left(1 - \frac{\alpha}{2}\right) \eta A, \quad Q = I - \frac{\eta}{2} A
\]

and \(K_m\) are the vectors of truncation errors at time \(t = t_m\). Define \(S = P^{-1}\) and \(R = SQ\). Then

\[
E_m = \alpha R E_{m-1} + \sum_{k=2}^{m-1} g_k^{(\alpha)} S E_{m-k} + SK_m.
\]

In Theorem \([29]\) we show that the vectors \(E_m\) converge to zero with second order accuracy with respect to \(h\) and \(\tau\).
Let $B = (b_{nm})$ be a square matrix of order $N - 1$. The maximum (infinity) norm of $B$ is defined as

$$\|B\| = \max_{1 \leq n \leq N-1} \sum_{m=1}^{N-1} |b_{nm}|$$

The vector and matrix norms satisfy

$$\|Bx\| \leq \|B\| \|x\|. \quad (61)$$

Let $\mu_1, \cdots, \mu_{N-1}$ be the eigenvalues of $B$. The spectral radius of $B$ is the maximum of the absolute values of its eigenvalues.

$$\rho(B) = \max_{1 \leq n \leq N-1} |\mu_n|.$$ 

The matrices $P, Q, R$ and $S$ are symmetric and commute, because the matrix $A$ is symmetric and definition (59). The matrix $P$ is a diagonally dominant M-matrix. Then the matrix $S = P^{-1}$ is positive and $\|S\| \leq 1$. The matrix $A$ has eigenvalues

$$\lambda_k = 4 \sin^2 \left( \frac{k\pi}{N} \right), \quad (k = 1, \cdots, N - 1).$$

The matrix $P$ has eigenvalues $1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k$, and the eigenvalues of the matrix $P^{-1}$ are

$$\left( 1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k \right)^{-1}.$$

Now we show that $R$ is a convergent matrix.

**Lemma 19.**

$$\rho(R) < 1.$$ 

**Proof.** The matrix $R = P^{-1}Q$ has eigenvalues,

$$\frac{1 - \frac{\eta \lambda_k}{2}}{1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k}.$$

Then

$$\left| \frac{1 - \frac{\eta \lambda_k}{2}}{1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k} \right| < 1, \quad \left| 1 - \frac{\eta \lambda_k}{2} \right| < \left| 1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k \right|,$$

$$\left( 1 - \frac{\eta \lambda_k}{2} \right)^2 < \left( 1 + \left( 1 - \frac{\alpha}{2} \right) \eta \lambda_k \right)^2,$$
\[ 1 - \eta \lambda_k + \frac{\eta^2(\lambda_k)^2}{4} < 1 + 2 \left(1 - \frac{\alpha}{2}\right) \eta \lambda_k + \left(1 - \frac{\alpha}{2}\right)^2 \eta^2(\lambda_k)^2, \]

\[ - \left(1 + 2 \left(1 - \frac{\alpha}{2}\right)\right) \eta \lambda_k < \left(\left(1 - \frac{\alpha}{2}\right)^2 - \frac{1}{4}\right) \eta^2(\lambda_k)^2, \]

\[ - (3 - \alpha) \eta \lambda_k < \frac{1}{4}(1 - \alpha)(3 - \alpha)\eta^2(\lambda_k)^2. \]

The above inequality holds because the left-hand side is negative and the right-hand side is positive. \( \square \)

The norm and the spectral radius of the matrix \( R \) satisfy

\[ \rho(R) < \|R\|. \]

While the norm of \( S \) is smaller than one, the norm of the matrix \( R \) may be greater than one. In the proof of Lemma 28 we use the following property of convergent matrices.

**Lemma 20.** There exists a positive integer \( J \) such that

\[ \| R^k S^{J-k} \| < 1 \]

for all \( 0 \leq k \leq J \).

**Proof.** The matrices \( R \) and \( S \) are convergent matrices. Then

\[ \lim_{k \to \infty} \| R^k \| = \lim_{k \to \infty} \| S^k \| = 0. \]

The sequence \( \{\| R^k \|\}_{k=0}^\infty \) is bounded. Let \( C_R \) be a positive constant such that

\[ \| R^k \| < C_R, \quad (k = 1, 2, \ldots) \]

and

\[ C_R > \max \left\{ K, \frac{5K}{(1-\alpha)2^\alpha} \right\}. \quad (62) \]

The number \( C_R \) is greater than one, because \( K > 1 \). Let \( J' \) be a positive integer such that

\[ \| R^k \| < 1, \quad \| S^k \| < \frac{1}{C_R}, \quad (k \geq J') \]

Choose \( J > 2J' \). When \( k \geq J' \) we have

\[ \| R^k S^{J-k} \| \leq \| R^k \| \| S^{J-k} \| \leq \| R^k \| \| S \|^{J-k} < 1. \]
If \( k < J' \) then \( J - k > J' \) and
\[
\| R^k S^{J-k} \| \leq \| R^k \| \| S^{J-k} \| < C_R \frac{1}{C_R} = 1.
\]

In addition we require that the number \( J \) is large enough such that the following inequality is satisfied
\[
(C_R)^J > (\alpha J C_R + 1) K.
\] (63)

Such number exists because \( C_R > K > 1 \) and the exponential function \((C_R)^J\) grows faster than the linear function \((\alpha J C_R + 1) K\). We use properties (62) and (63) of the numbers \( C_R \) and \( J \) in Corollary 25 and Lemma 26. Denote
\[
\Phi_m^{(0)} = \sum_{k=2}^{m-1} g_k^{(0)} S E_{m-k}.
\]
The vectors \( E_m \) and \( E_{m-1} \) are computed recursively as
\[
E_m = \alpha R E_{m-1} + \Phi_m^{(0)} + S K_m,
\] (64)
\[
E_{m-1} = \alpha R E_{m-2} + \Phi_{m-1}^{(0)} + S K_{m-1}.
\]
Then
\[
E_m = \alpha R \left( \alpha R E_{m-2} + \Phi_{m-1}^{(0)} + S K_{m-1} \right) + \Phi_m^{(0)} + S K_m,
\]
\[
E_m = \alpha^2 R^2 E_{m-2} + \sum_{k=2}^{m-2} \alpha g_k^{(0)} R S E_{m-k-1} + \Phi_m^{(0)} + \alpha R S K_{m-1} + S K_m.
\] (65)

In Lemma 21 we define the numbers \( \beta_{n,k,i}^{(m)} \) and the vectors \( A_{m,n} \) recursively with (66), (67) and (68). The boundary values of \( \beta_{n,k,i}^{(m)} \) and \( A_{m,n} \) are
\[
\begin{cases}
\beta_{n,0,m-n}^{(m)} = \alpha^n, & m \geq 1, \\
\beta_{n,0,i}^{(m)} = 0, & i \neq m - n, \\
\beta_{n,k,i}^{(m)} = 0, & k < 0, k \geq n,
\end{cases}
\]
\[
A_{m,0} = S K_m, \quad A_{m,1} = \alpha R S K_{m-1} + S K_m.
\]
Lemma 21. There exist positive numbers $\beta_{n,k,i}^{(m)}$ such that the error vector $E_m$ can be represented as

$$E_m = \alpha^n R^n E_{m-n} + \sum_{k=1}^{n-1} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} R^{n-k} S^k E_i + \Phi_m^{(\alpha)} + A_{m,n}. \quad (66)$$

The numbers $\beta_{n,k,i}^{(m)}$ and the vectors $A_{m,n}$ are computed recursively as

$$\beta_{n+1,k,i}^{(m)} = \alpha \beta_{n,k,i}^{(m)} + \sum_{j=2}^{m-n-k-i+1} g_j^{(\alpha)} \beta_{n,k,j+i}^{(m)}, \quad (67)$$

$$A_{m+1,n} = A_{m,n} + \alpha^n R^n S K_{m-n} + \sum_{k=1}^{n-1} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} R^{n-k} S^{k+1} K_i. \quad (68)$$

Proof. We prove that (67) and (68) hold by induction on $n$. From the definition of $\beta_{n,k,i}^{(m)}$, $A_{m,n}$ and formulas (64) and (65) we have that (67) and (68) hold for $n = 1$ and $n = 2$. Suppose that (67) and (68) hold for all $n \leq \bar{n}$. Then

$$E_m = \alpha^n R^n E_{m-\bar{n}} + \sum_{k=1}^{\bar{n}-1} \sum_{i=1}^{m-\bar{n}-k} \beta_{\bar{n},k,i}^{(m)} R^{\bar{n}-k} S^k E_i + \Phi_m^{(\alpha)} + A_{m,\bar{n}}.$$

By substituting the vectors $E_1, E_2, \ldots, E_{m-\bar{n}}$ with (60) we get

$$E_m = \alpha^{\bar{n}} R^{\bar{n}} E_{m-\bar{n}} + \sum_{k=1}^{\bar{n}-1} \sum_{i=1}^{m-\bar{n}-k} \beta_{\bar{n},k,i}^{(m)} R^{\bar{n}-k} S^k E_i + \Phi_m^{(\alpha)} + A_{m,\bar{n}}$$

$$+ \sum_{k=1}^{\bar{n}-1} \sum_{i=1}^{m-\bar{n}-k} \beta_{\bar{n},k,i}^{(m)} R^{\bar{n}-k} S^k \left( \alpha RE_{i-1} + \sum_{k=2}^{i-1} g_k^{(\alpha)} S E_{i-k} + SK_i \right). \quad (69)$$

The formula for recursive computation (68) of the vectors $A_{m,\bar{n}}$ of approximation errors is obtained from (69) as the sum of the approximation errors. The coefficient of $R^{\bar{n}+1-k} S^k$ in formula (60) with $n = \bar{n} + 1$

$$\sum_{i=1}^{m-\bar{n}-k-1} \beta_{\bar{n}+1,k,i}^{(m)} E_i$$

is determined from the coefficients of $R^{\bar{n}-k} S^k$ and $R^{\bar{n}+1-k} S^{k-1}$ in (69) with $n = \bar{n}$. The coefficient of $R^{\bar{n}-k} S^k$ is

$$\sum_{i=1}^{m-\bar{n}-k} \beta_{\bar{n},k,i}^{(m)} E_i.$$

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After one iteration the coefficient becomes
\[ \sum_{i=1}^{m-k} \alpha \beta^{(m)}_{n,k,i} E_{i-1} = \sum_{i=1}^{m-k-1} \alpha \beta^{(m)}_{n,k,i+1} E_i. \]

Similarly, the coefficient of \( R^{k+1} S^{k-1} \) is initially
\[ \sum_{i=1}^{m-k+1} \beta^{(m)}_{n,k-1,i} E_i. \]

After one iteration it becomes
\[ \sum_{i=1}^{m-k+1} \beta^{(m)}_{n,k-1,i} \sum_{j=2}^{i-1} g_j^{(a)} E_{i-j} = \sum_{i=1}^{m-k+1} \sum_{j=2}^{i-1} g_j^{(a)} \beta^{(m)}_{n,k-1,i} E_{i-j}. \]

By substituting \( l = i - j \) we obtain
\[ \sum_{i=3}^{m-k+1} \sum_{j=2}^{i-1} g_j^{(a)} \beta^{(m)}_{n,k-1,i} E_{i-j} = \sum_{i=1}^{m-k+1} \sum_{j=2}^{m-k-l} g_j^{(a)} \beta^{(m)}_{n,k-1,j+i} E_i. \] (70)

Then
\[ \sum_{i=1}^{m-k-1} \beta^{(m)}_{n+1,k,i} E_i = \sum_{i=1}^{m-k-1} \alpha \beta^{(m)}_{n,k,i+1} E_i + \sum_{i=1}^{m-k-1} \sum_{j=2}^{m-k-i} g_j^{(a)} \beta^{(m)}_{n,k-1,j+i} E_i, \]
\[ \sum_{i=1}^{m-k-1} \beta^{(m)}_{n+1,k,i} E_i = \sum_{i=1}^{m-k-1} \left( \alpha \beta^{(m)}_{n,k,i+1} + \sum_{j=2}^{m-k-i} g_j^{(a)} \beta^{(m)}_{n,k-1,j+i} \right) E_i. \]

The coefficients of \( E_i \) are equal. Therefore
\[ \beta^{(m)}_{n+1,k,i} = \alpha \beta^{(m)}_{n,k,i+1} + \sum_{j=2}^{m-k-i} g_j^{(a)} \beta^{(m)}_{n,k-1,j+i}. \]

We use (67) for recursive computation of all coefficients \( \beta^{(m)}_{n+1,k,i} \) for \( k = 1, \ldots, n - 1 \). The formula also holds in the boundary cases \( k = 0 \) and \( k = n \).

When \( k = 0 \) we have,
\[ \beta^{(m)}_{n+1,0,i} = \alpha \beta^{(m)}_{n,0,i+1} + \sum_{j=2}^{m-n-k-1} g_j^{(a)} \beta^{(m)}_{n-1,j+i} = \alpha \beta^{(m)}_{n,0,i+1} \]

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because $\beta_{n-1,j+i}^{(m)} = 0$. Then
\[
\beta_{n+1,0,m-n-1}^{(m)} = \alpha \beta_{n,0,m-n}^{(m)} = \alpha^{n+1}.
\]

When $k = n$,
\[
\beta_{n+1,n,i}^{(m)} = \alpha \beta_{n,n+1,i}^{(m)} + \sum_{j=2}^{m-2n-i+1} g_j^{(\alpha)} \beta_{n,n-1,j+i}^{(m)} = \sum_{j=2}^{m-2n-k-i+1} g_j^{(\alpha)} \beta_{n,n-1,j+i}^{(m)}.
\]

A more convenient way to write formulas (66) and (68) is
\[
E_m = \sum_{k=0}^{n-1} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} R^{n-k} S^k E_i + \Phi^{(\alpha)}(m) + A_{m,n}, \quad (71)
\]
\[
A_{m,n+1} = A_{m,n} + \sum_{k=0}^{n-1} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} R^{n-k} S^{k+1} K_i.
\]

Denote,
\[
\tilde{\beta}_n^{(m)} = \sum_{k=0}^{n-1} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)}.
\]

**Corollary 22.** The sequence $\tilde{\beta}_n^{(m)}$ is decreasing.

**Proof.**

\[
\tilde{\beta}_{n+1}^{(m)} = \sum_{k=0}^{n} \sum_{i=1}^{m-n-k} \beta_{n,k,i+1}^{(m)} = \sum_{k=0}^{n} \left( \alpha \sum_{i=1}^{m-n-k-1} \beta_{n,k,i+1}^{(m)} + \sum_{i=1}^{m-n-k-1} \sum_{j=2}^{m-n-k-i+1} g_j^{(\alpha)} \beta_{n,k-1,j+i}^{(m)} \right).
\]

Substitute $l = i + j$.

\[
\tilde{\beta}_{n+1}^{(m)} = \sum_{k=0}^{n} \left( \alpha \sum_{i=1}^{m-n-k-1} \beta_{n,k,i+1}^{(m)} + \sum_{i=3}^{m-n-k} \sum_{l=2}^{i-1} \beta_{n,k-1,i}^{(m)} g_l^{(\alpha)} \right).
\]

We have that
\[
\sum_{l=2}^{i-1} g_l^{(\alpha)} < \sum_{l=2}^{\infty} g_l^{(\alpha)} = 1 - \alpha.
\]

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Then
\[ \tilde{\beta}_{n+1}^{(m)} < \sum_{k=0}^{n} \left( \alpha \sum_{i=2}^{m-n-k} \beta_{n,k,i}^{(m)} + (1 - \alpha) \sum_{i=3}^{m-n-k} \beta_{n,k,i}^{(m)} \right), \]
\[ \tilde{\beta}_{n+1}^{(m)} < \sum_{k=0}^{n} \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} = \tilde{\beta}_{n}^{(m)}. \]

The value of \( \tilde{\beta}_1^{(m)} \) is
\[ \tilde{\beta}_1^{(m)} = \sum_{i=1}^{m-1} \beta_{1,0,i} = \beta_{1,0,m-1} = \alpha. \]

**Corollary 23. (Estimate for sums of coefficients of (71))**
\[ \sum_{k=0}^{n-1} m-n-k \sum_{i=1}^{m-n-k} \beta_{n,k,i}^{(m)} < \alpha. \]

**Proof.** The sequence \( \{\tilde{\beta}_{n}^{(m)}\} \) is decreasing. Then
\[ \beta_{n}^{(m)} < \tilde{\beta}_1^{(m)} = \alpha. \]

**Lemma 24. (Estimate for the norm of \( A_{m,n} \))**
\[ \|A_{m,n}\| \leq (n\alpha C_R + 1)K\tau^\alpha \left( \tau^2 + h^2 \right). \] (72)

**Proof.** When \( n = 1 \) we have
\[ A_{m,1} = \alpha RSK_{m-1} + SK_m, \]
\[ \|A_{m,1}\| \leq \alpha \|R\| \|S\| \|K_{m-1}\| + \|S\| \|K_m\| \leq (\alpha C_R + 1)K\tau^\alpha \left( \tau^2 + h^2 \right). \]

We prove (72) by induction on \( n \). Suppose that (72) holds for \( n \leq \pi \). The vectors \( A_{m,\pi} \) are computed recursively with
\[ A_{m,\pi+1} = A_{m,\pi} + \sum_{k=0}^{\pi-1} m-\pi-k \sum_{i=1}^{\beta_{\pi,k,i}^{(m)}} R^{\pi-k} S^{k+1} K_i. \]

Then
\[ \|A_{m,\pi+1}\| \leq \|A_{m,\pi}\| + \sum_{k=0}^{\pi-1} m-\pi-k \sum_{i=1}^{\beta_{\pi,k,i}^{(m)}} \|R^{\pi-k}\| \|S^{k+1}\| \|K_i\|, \]

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\[ \|A_{m,n+1}\| \leq \|A_{m,n}\| + KC_R \tau^\alpha (\tau^2 + h^2) \sum_{k=0}^{n-1} \sum_{i=1}^{m-1-k} \beta_{m,k,i}^{(n)}. \]

From Corollary 23 and the induction hypothesis
\[ \|A_{m,n+1}\| \leq \|A_{m,n}\| + \alpha KC_R \tau^\alpha (\tau^2 + h^2), \]
\[ \|A_{m,n+1}\| \leq (n\alpha C_R + 1) K \tau^\alpha (\tau^2 + h^2), \]
\[ \|A_{m,n+1}\| \leq ((\pi + 1)\alpha C_R + 1) K \tau^\alpha (\tau^2 + h^2). \]

By setting \( n = J \), where \( J \) is the number determined in Lemma 20 and (63), and combining the results from Corollary 23 and Corollary 24 we obtain.

**Corollary 25.** The vectors \( E_m \) are computed recursively with
\[ E_0 = 0 \]
\[ E_m = \sum_{k=0}^{J-1} \sum_{i=1}^{J-k} \beta_{J,k,i}^{(m)} R_{j-k} S_k E_i + \sum_{k=2}^{m-1} g_k^{(\alpha)} SE_{m-k} + A_{m,J}, \]
where the numbers \( \beta_{J,k,i}^{(m)} \geq 0 \), \( g_k^{(\alpha)} > 0 \) and the vectors \( A_{m,J} \) satisfy
\[ \sum_{k=0}^{J-1} \sum_{i=1}^{J-k} \beta_{J,k,i}^{(m)} + \sum_{k=2}^{m-1} g_k^{(\alpha)} < \sum_{k=1}^{m-1} g_k^{(\alpha)}, \]
\[ \|A_{m,J}\| \leq (\alpha J C_R + 1) K \tau^\alpha (\tau^2 + h^2) < C_R^J \tau^\alpha (\tau^2 + h^2). \]

In the next two lemmas we determine estimates for the error vectors \( E_m \).

**Lemma 26.** Let \( m \leq J \). Then
\[ \|E_m\| < (C_R)^m \tau^\alpha (\tau^2 + h^2). \]

**Proof.** Induction on \( m \):
\[ E_1 = \alpha RE_0 + SK_1 = SK_1, \]
\[ \|E_1\| \leq \|SK_1\| \leq \|S\| \|K_1\| \leq \|K_1\| < K \tau^\alpha (\tau^2 + h^2) < C_R \tau^\alpha (\tau^2 + h^2). \]

Suppose that (75) holds for \( m < \pi \). The vector \( E_{\pi} \) is computed recursively with
\[ E_{\pi} = \alpha RE_{\pi-1} + \sum_{k=2}^{\pi-1} g_k^{(\alpha)} SE_{\pi-k} + SK_{\pi}. \]
Then
\[ \|E_m\| \leq \alpha \|R\| + \|E_{m-1}\| + \sum_{k=2}^{m-1} g_k^{(\alpha)} \|S\| \|E_{m-k}\| + \|S\| \|K_{m}\|, \]

\[ \|E_m\| \leq \alpha C_R \|E_{m-1}\| + \sum_{k=2}^{m-1} g_k^{(\alpha)} \|E_{m-k}\| + \|K_m\|. \]

By the induction hypothesis
\[ \|E_{m-k}\| < (C_R)^{m-k} (m-k)^\alpha (\tau^2 + h^2) \leq (C_R)^{m-1} \|E_{m-k}\| \leq \alpha \tau^2 + h^2. \]

Then
\[ \frac{\|E_m\|}{\tau^\alpha (\tau^2 + h^2)} < \alpha (C_R)^{m\alpha} + (C_R)^{m-1} \sum_{k=2}^{m-1} g_k^{(\alpha)} + K, \]

\[ \frac{\|E_m\|}{\tau^\alpha (\tau^2 + h^2)} < \alpha (C_R)^{m\alpha} + (C_R)^{m-1} \sum_{k=2}^{\infty} g_k^{(\alpha)} - (C_R)^{m-1} \sum_{k=m}^{\infty} g_k^{(\alpha)} + K. \]

From Lemma 12,
\[ \sum_{k=m}^{\infty} g_k^{(\alpha)} > \frac{1 - \alpha}{5} \frac{2^\alpha}{m^\alpha}. \]

Then
\[ \frac{\|E_m\|}{\tau^\alpha (\tau^2 + h^2)} < \alpha (C_R)^{m\alpha} + (1 - \alpha)(C_R)^{m\alpha} - C_R \cdot \frac{1 - \alpha}{5} \frac{2^\alpha}{m^\alpha} + K. \]

\[ \frac{\|E_m\|}{\tau^\alpha (\tau^2 + h^2)} < (C_R)^{m\alpha} - \frac{(1 - \alpha)2^\alpha}{5} C_R + K. \]

Hence,
\[ \|E_m\| \leq (C_R)^{m\alpha} \tau^\alpha (\tau^2 + h^2). \]

because \( C_R > 5K/((1 - \alpha)2^\alpha). \)

**Corollary 27.** Let \( m \leq J. \) Then
\[ \|E_m\| \leq (C_R)^J m^\alpha \tau^\alpha (\tau^2 + h^2). \]
Lemma 28. (Estimate for the vectors $E_m$)

$$
\| E_m \| < C m^\alpha \tau^\alpha \left( \tau^2 + h^2 \right),
$$

where

$$
C = \max \left\{ (C_R)^J, \frac{5 (C_R)^J}{(1 - \alpha)} \right\}.
$$

Proof. Induction on $m$. From Corollary 27 estimate (76) holds for $m \leq J$. Suppose that (76) holds for $m < \overline{m}$, where $\overline{m} > J$. The vector $E_{\overline{m}}$ is computed recursively with

$$
E_{\overline{m}} = \sum_{k=0}^{J-1} \sum_{i=1}^{\overline{m} - J - k} \beta_{J,k,i}^{(m)} R^{J-k} S^{k} E_i + \sum_{k=2}^{\overline{m} - 1} g_k^{(\alpha)} S E_{\overline{m} - k} + A_{\overline{m},J}.
$$

Then

$$
\| E_{\overline{m}} \| \leq \sum_{k=0}^{J-1} \sum_{i=1}^{\overline{m} - J - k} \beta_{J,k,i}^{(m)} \| R^{J-k} S^k \| \| E_i \| + \sum_{k=2}^{\overline{m} - 1} g_k^{(\alpha)} \| S \| \| E_{\overline{m} - k} \| + \| A_{\overline{m},J} \|.
$$

The number $J$ is chosen in Lemma 20 such that $\| R^{J-k} S^k \| < 1$. Then

$$
\| E_{\overline{m}} \| < \sum_{k=0}^{J-1} \sum_{i=1}^{\overline{m} - J - k} \beta_{J,k,i}^{(m)} \| E_i \| + \sum_{k=2}^{\overline{m} - 1} g_k^{(\alpha)} \| E_{\overline{m} - k} \| + \| A_{\overline{m},J} \|.
$$

By the inductive hypothesis

$$
\| E_{\overline{m} - k} \| < C (\overline{m} - k)^\alpha \tau^\alpha \left( \tau^2 + h^2 \right) < C\overline{m}^\alpha \tau^\alpha \left( \tau^2 + h^2 \right).
$$

Then

$$
\| E_{\overline{m}} \| < C\overline{m}^\alpha \tau^\alpha \left( \tau^2 + h^2 \right) \left( \sum_{k=0}^{J-1} \sum_{i=1}^{\overline{m} - J - k} \beta_{J,k,i}^{(m)} + \sum_{k=2}^{\overline{m} - 1} g_k^{(\alpha)} \right) + (C_R)^J \tau^\alpha \left( \tau^2 + h^2 \right).
$$

From (74),

$$
\| E_{\overline{m}} \| < C\overline{m}^\alpha \tau^\alpha \left( \tau^2 + h^2 \right) \sum_{k=1}^{\overline{m} - 1} g_k^{(\alpha)} + (C_R)^J \tau^\alpha \left( \tau^2 + h^2 \right),
$$

$$
\frac{\| E_{\overline{m}} \|}{\tau^\alpha \left( \tau^2 + h^2 \right)} < C\overline{m}^\alpha \left( \sum_{k=1}^{\overline{m}} g_k^{(\alpha)} - \sum_{k=\overline{m}}^{\infty} g_k^{(\alpha)} \right) + (C_R)^J.
$$
We have that
\[ \sum_{k=1}^{\infty} g_k^{(\alpha)} = 1, \quad \sum_{k=m}^{\infty} g_k^{(\alpha)} > \frac{1 - \alpha}{5} \left( \frac{2}{m} \right)^{\alpha}. \]

Then
\[ \frac{\| E_m \|}{\tau^\alpha (\tau^2 + h^2)} < C m^\alpha - Cm^\alpha \frac{1 - \alpha}{5} \left( \frac{2}{m} \right)^{\alpha} + (C_R)^J, \]
\[ \frac{\| E_m \|}{\tau^\alpha (\tau^2 + h^2)} < C m^\alpha - \frac{(1 - \alpha)2^\alpha}{5} C + (C_R)^J, \]
\[ \| E_m \| < C m^\alpha \tau^\alpha \left( \tau^2 + h^2 \right), \]
because \( C > 5(C_R)^J/((1 - \alpha)2^\alpha). \)

**Theorem 29.** Difference approximations (56) and (57) are unconditionally stable and converge to the solution of (53) with second order accuracy with respect to the space and time variables.

**Proof.** The value of \( \tau \) is \( \tau = T/M \). From Lemma 28,

\[ \| E_m \| < C m^\alpha \tau^\alpha \left( \tau^2 + h^2 \right) \leq C T^\alpha \left( \frac{m}{M} \right)^{\alpha} \left( \tau^2 + h^2 \right), \]
\[ \| E_m \| < C T^\alpha \left( \tau^2 + h^2 \right). \]

for all \( m \leq M. \)

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