THE θ-SCHEME FOR CAPUTO FRACTIONAL DIFFERENTIAL EQUATIONS

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ABSTRACT. The θ-numerical scheme is formulated for Caputo fractional differential equations (FDEs) of order $\alpha \in (0, 1)$ with vector fields satisfying a standard Lipschitz continuity condition in the state variable and a Hölder continuity condition in the time variable. The convergence rate is established and a numerical example is given to illustrate the theoretical results. The scheme obtained includes the explicit ($\theta = 0$) and implicit (θ =1) counterparts of Euler-like schemes for Caputo FDEs known in the literature as the Adams-Bashford and Adams-Moulton schemes, respectively, and essentially linearly interpolates them.

Caputo fractional differential equations, theta scheme, Euler scheme, Adams-Bashford scheme, Adams-Moulton scheme.
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1. INTRODUCTION

Fractional order differential equations are suitable for describing various complex phenomena, in particular memory and hereditary properties of dynamical processes, see the monographs [3, 11, 26] and the references therein. An extensive qualitative theory of such equations is now available (see e.g., [3, 5, 11, 15, 24, 26]. Explicit solutions are rarely known and then often have complicated expressions, which are of little practical use. Numerical methods have been developed over many decades for equations containing derivatives and integrals of non-integer order. More specifically, numerical methods for fractional differential equations have been considered by many authors [4, 6, 7, 8, 9, 10, 11, 14, 16, 17, 22, 23, 24, 25]. These results and many more are discussed in the monographs [20, 21, 23]. Of particular interest here are the fractional Adams-Bashforth/Moulton methods developed by Diethelm et al [8, 9, 11], which are essentially the Caputo counterparts of the explicit/implicit Euler schemes.

The Euler scheme is the simplest numerical scheme for a first-order ordinary differential equation (ODEs) with the vector field $f(t, x)$ and is easily derived due to the geometric interpretation of the classical derivative. The θ-scheme essentially linearly interpolates the explicit ($\theta = 0$) and implicit ($\theta = 1$) versions of the Euler scheme, specifically

$$x^{(n)}(t_{n+1}) = x^{(n)}(t_n) + (1-\theta)f(t_n, x^{(n)}(t_n))h + \theta f(t_n, x^{(n)}(t_{n+1}))h \quad (1)$$

for a time step $h > 0$ and parameter $0 \le \theta \le 1$. Here, $t_n = nh$. It is implicit except when $\theta = 0$. This scheme is now finding increasing use, especially when numerical stability is an issue [19].

The piecewise linear interpolation $x^{(n)}(t)$ of the iterates of the θ-scheme can be expressed in integral form as

$$x^{(n)}(t) = x_0 + (1-\theta)\int_0^t f(\zeta_n(s), x^{(n)}(\zeta_n(s)))\, ds + \theta \int_0^t f(\lambda_n(s), x^{(n)}(\lambda_n(s)))\, ds, \quad (2)$$

where $\zeta_n(s) = \frac{kT}{n}$ and $\lambda_n(s) = \frac{(k+1)T}{n}$ for $s \in \left(\frac{kT}{n}, \frac{(k+1)T}{n}\right]$, $k = 0, \ldots, n-1$.

Now consider a Caputo FDEs of order $\alpha \in (0,1)$ on the interval $[0,T]$ of the form

$$^{C}D^{\alpha}_{0+}Y(t) = f(t, Y(t)), \quad (3)$$

with the same vector field $f : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$. This has the integral equation representation

$$Y(t) \;=\; y_0 + \frac{1}{\Gamma(\alpha)}\int_0^t \frac{f(s, Y(s))}{(t-s)^{1-\alpha}}\, ds, \quad (4)$$

where Γ is the Gamma function, i.e., $\Gamma(\alpha) := \int_0^\infty s^{\alpha-1}e^{-s}\, ds$.

This and the integral expression (2) suggest the following definition of the piecewise linear interpolation $y^{(n)}(t)$ of the *θ-scheme* for the Caputo FDEs (3):

$$\begin{aligned} Y^{(n)}(t) \;=\; & y_0 + \frac{(1-\theta)}{\Gamma(\alpha)}\int_0^t \frac{f(\zeta_n(s), Y^{(n)}(\zeta_n(s)))}{(t-s)^{1-\alpha}}\, ds \\ & + \frac{\theta}{\Gamma(\alpha)}\int_0^t \frac{f(\lambda_n(s), Y^{(n)}(\lambda_n(s)))}{(t-s)^{1-\alpha}}\, ds \end{aligned} \quad (5)$$

for $t \in [0,T]$. Indeed, this approach was used by the authors [14] to define the Euler-Maruyama scheme for Caputo fractional stochastic differential equations.

The θ- scheme (5) can be written step by step on each interval $\left(\frac{kT}{n}, \frac{(k+1)T}{n}\right]$, $k = 0, \ldots, n-1$. Write $Y^{(n)}_k = Y^{(n)}(\frac{kT}{n})$ with $Y^{(n)}_0$

$= y_0$. Then,

$$
\begin{aligned}
& Y_{k+1}^{(n)} \\
= \;& Y_0^{(n)} + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^{k} \Big[\, (1-\theta) f(t_j, Y_j^{(n)}) + \theta f(t_{j+1}, Y_{j+1}^{(n)}) \Big] \int_{t_j}^{t_{j+1}} \frac{1}{(t_{k+1}-s)^{1-\alpha}} \, ds \\
= \;& Y_0^{(n)} + \frac{1}{\alpha \Gamma(\alpha)} \sum_{j=0}^{k} \Big[\, (1-\theta) f(t_j, Y_j^{(n)}) + \theta f(t_{j+1}, Y_{j+1}^{(n)}) \Big] \left((t_{k+1}-t_j)^\alpha - (t_{k+1}-t_{j+1})^\alpha \right) \\
= \;& Y_0^{(n)} + \frac{1}{\Gamma(\alpha+1)} \sum_{j=0}^{k} \Big[(1-\theta) f(t_j, Y_j^{(n)}) + \theta f(t_{j+1}, Y_{j+1}^{(n)}) \Big] \; \left((k+1-j)^\alpha - (k-j)^\alpha \right) \left(\frac{T}{n} \right.
\end{aligned}
$$

This gives the recursive formula

$$
Y_{k+1}^{(n)} = Y_0^{(n)} + \sum_{j=0}^{k} \gamma_{k-j} \Big[(1-\theta) f(t_j, Y_j^{(n)}) + \theta f(t_{j+1}, Y_{j+1}^{(n)}) \Big] \left(\frac{T}{n} \right)^{\alpha}, \tag{6}
$$

for $k = 0, \ldots, n-1$ and

$$
\gamma_j := \frac{1}{\Gamma(\alpha+1)} \; \left((j+1)^\alpha - j^\alpha \right).
$$

Note that γ_j decreases from $\gamma_0 = \frac{1}{\Gamma(\alpha+1)}$ as j increases, i.e., the weighting of the contribution of $f(t_j, Y_j^{(n)})$ and $f(t_{j+1}, Y_{j+1}^{(n)})$ for a given j decreases as n increases.

This scheme (6) is known in the literature as the Adams-Bashford scheme for $\theta = 0$ and Adams-Moulton scheme for $\theta = 1$ as the [9, 10, 11]. These are the counterparts of the explicit and implicit Euler schemes for Caputo FDEs. They were also given without derivation or error bound in [16, p. 19].

When $\alpha = 1$, in which case the weights $\gamma_j \equiv 1$, the expression (6) reduces to θ -scheme (1) for ordinary differential equations (ODEs). For simplicity this will be shown for the case $\theta = 0$.

$$
Y_{k+1}^{(n)} = Y_0^{(n)} + \sum_{j=0}^{k} \; f(t_j, Y_j^{(n)}) \, \frac{T}{n}, \quad k = 0, \ldots, n-1,
$$

which gives

$$
\begin{aligned}
Y_1^{(n)} &= Y_0^{(n)} + f(t_0, Y_0^{(n)}) \, \frac{T}{n}, \\
Y_2^{(n)} &= Y_0^{(n)} + f(t_0, Y_0^{(n)}) \, \frac{T}{n} + f(t_1, Y_1^{(n)}) \, \frac{T}{n} = Y_1^{(n)} + f(t_1, Y_1^{(n)}) \, \frac{T}{n},
\end{aligned}
$$

and so on, culminating in

$$Y_{k+1}^{(n)} = Y_k^{(n)} + f(t_k, Y_k^{(n)})\,\frac{T}{n}.$$

The case $\theta = 1$ and the general case are similar.

The paper is organized as follows. In Section 2, we give a setting of the problem and state the main result of the paper (Theorem 2.1) on θ-scheme. Section 3 is devoted to proving the main result. Finally, in Section 4, a simple example is studied numerically.

2. Main result

Fix $T > 0$ arbitrarily and consider the Caputo FDEs (3) of order $\alpha \in (0,1)$ on the interval $[0,T]$ where $f : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ satisfies the following conditions

(H1) *Lipschitz continuity with respect to the second variable*: There exists $L_1 > 0$ such that for all $y, y_1 \in \mathbb{R}^d, t \in [0,T]$,

$$\|f(t,y) - f(t,y_1)\| \le L_1\|y - y_1\|.$$

(H2) *Hölder continuity with respect to the first variable*: There exists $L_2 > 0$ and $\beta \in [0,1]$ such that for all $y \in \mathbb{R}^d$, $t, t_1 \in [0,T]$

$$\|f(t,y) - f(t_1,y)\| \le L_2|t - t_1|^\beta.$$

As a consequence, the function f also satisfies a linear growth bound

$$\|f(t,y)\| \le M + L_1\|y\|, \quad y \in \mathbb{R}^d, t \in [0,T], \tag{7}$$

with $M := \max_{t\in[0,T]} \|f(t,0)\|$.

Then, (3) with the initial value $Y(0) = y_0 \in \mathbb{R}^d$ has a unique solution on $[0,T]$ denoted by $Y(t)$, which satisfies the integral representation (4) (see e.g., [2, Theorem 2] and [27, Theorem 6.4]). Notice that the kernel $(t-s)^{\alpha-1}$ of (4) is singular at the point $s = t$, but integrable.

The first part of the following result shows that the θ-scheme (5) is uniquely solvable when the step size is small enough. The second part establishes a global discretization error between the numerical solution $Y^{(n)}(t)$ and the exact solution $Y(t)$ of the Caputo FDEs (3).

Theorem 2.1 (Solvability and convergence of the θ-scheme (5) for Caputo FDEs)**.** *Suppose that Assumptions* (H1) *and* (H2) *hold and let N be the smallest natural number satisfying that*

$$N \ge T\,\sqrt[\alpha]{\frac{2\,\theta\,L_1}{\Gamma(\alpha+1)}}, \tag{8}$$

where L_1 is the constant in Assumption (H1). Then, the following statements hold:

(i) *For any $n \ge N$, equation* (5) *has a unique solution $Y^{(n)}(t_{k+1})$ with $Y^{(n)}(0) := y_0$ for each $k = 0, \dots, n-1$.*

(ii) *There exists a constant* C *depending only on* $\theta, y_0, T, L_1, L_2, M, \alpha, \beta$ *such that*

$$\sup_{0\le t\le T} \|Y^{(n)}(t) - Y(t)\| \le \frac{C}{n^{\kappa}} \qquad \text{for all } n \ge N, \tag{9}$$

where $\kappa := \min\{\alpha, \beta\}$.

Remark 2.2. Similar results have been given by Diethelm [11, Appendix C] for the Adams-Bashford scheme ($\theta = 0$) and the Adams-Moulton scheme ($\theta = 1$). When $\alpha = 1$, i.e., (3) becomes an ODEs, the convergence rate of the scheme in Theorem 2.1 coincides with the well-known convergence rate of the explicit and implicit Euler schemes for ODEs (with $\theta = 0$ and $\theta = 1$, respectively) (see e.g., [1]).

3. Proof of the main result

First we prove solvability of the θ-scheme (5), which is implicit for $0 < \theta \le 1$.

Proof of Theorem 2.1 (i). Choose and fix an arbitrary natural number n such that

$$n \ge T \sqrt[\alpha]{\frac{2\,\theta\,L_1}{\Gamma(\alpha+1)}}, \tag{10}$$

where L_1 is the constant given in Assumption (H1). The $Y^{(n)}(t_0), \dots, Y^{(n)}(t_{n-1})$ are obtained inductively by solving the equations

$$Y^{(n)}(t_{k+1}) = y_0 + (1-\theta)\sum_{j=0}^{k} \gamma_{k-j}\, f(t_j, Y^{(n)}(t_j)) \left(\frac{T}{n}\right)^{\alpha} + \theta \sum_{j=0}^{k} \gamma_{k-j}\, f(t_{j+1}, Y^{(n)}(t_{j+1})) \left(\frac{T}{n}\right)^{\alpha}. \tag{11}$$

Obviously, $Y^{(n)}(t_0) = y_0$, so assume that the $Y^{(n)}(t_0), \dots, Y^{(n)}(t_j)$ have been determined for some $j \in \{0, \dots, n-2\}$. It needs to be shown that there is a unique solution $Y^{(n)}(t_{k+1})$ of the equation (11). For this purpose, define the map $\varphi : \mathbb{R}^d \to \mathbb{R}^d$ by

$$\begin{aligned}\varphi(x) \;&=\; x - \theta\,\gamma_0\, f(t_{k+1}, x)\left(\frac{T}{n}\right)^{\alpha} - y_0 - (1-\theta)\sum_{j=0}^{k} \gamma_{k-j}\, f(t_j, Y^{(n)}(t_j)) \left(\frac{T}{n}\right)^{\alpha}\\ &\quad -\theta\sum_{j=0}^{k-1} \gamma_{k-j}\, f(t_{j+1}, Y^{(n)}(t_{j+1}))\left(\frac{T}{n}\right)^{\alpha}.\end{aligned}$$

For arbitrary $x, y \in \mathbb{R}^d$, we have

$$\|\varphi(x) - \varphi(y)\| \;=\; \theta\,\gamma_0 \left(\frac{T}{n}\right)^{\alpha} \|f(t_{k+1}, x) - f(t_{k+1}, y)\| \le \theta\,\gamma_0 \left(\frac{T}{n}\right)^{\alpha} L_1 \|x - y\|,$$

where we used Assumption (H1) to obtain the last inequality. From (10), we derive that

$$\theta\,\gamma_0 \left(\frac{T}{n}\right)^{\alpha} L_1 = \frac{\theta}{\Gamma(\alpha+1)} \left(\frac{T}{n}\right)^{\alpha} L_1 < 1.$$

Therefore, the map φ is contractive. Using the Banach fixed point theorem, there exists a unique fixed point of this map in $\mathbb{R}^d$. □

In the rest of this section, we will prove the Theorem 2.1(ii). Our first task is to deduce from (5) an upper bound for $\sup_{0\le t\le T}\|Y^{(n)}(t)\|$. Since $Y^{(n)}(t)$ is constructed implicitly, the version of Gronwall's inequality for FDEs stated in [11, Lemma 6.19] (also in Dixon [12]) is not applicable. To overcome this difficulty, we use the weight function $E_\alpha(\mu\, t^\alpha)$, the increasing monotonicity of the Mittag-Leffler function $E_\alpha(\cdot)$ on $[0,\infty)$, and some skillful transformations. Here, the Mittag-Leffler function $E_\alpha : \mathbb{R} \to \mathbb{R}$ is defined by

$$E_\alpha(t) := \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\alpha k+1)}, \quad t\in\mathbb{R},\ \alpha\in(0,1).$$

An upper bound for the approximate solution is presented in the following lemma.

Lemma 3.1. *Let $n\in\mathbb{N}$ satisfy $n \ge T\sqrt[\alpha]{\frac{2\theta\, L_1}{\Gamma(\alpha+1)}}$ and define*

$$C_1 := \left(2\|y_0\| + \frac{2M(1+\theta)\,T^\alpha}{\Gamma(\alpha+1)}\right)\frac{\mu\, E_\alpha(\mu\, T^\alpha)}{\mu - 2L1}. \tag{12}$$

Then,

$$\sup_{0\le t\le T}\|Y^{(n)}(t)\| \le C_1. \tag{13}$$

Proof. Using (5), and the inequality $\|y_1+y_2+y_3+y_4\| \le \|y_1\|+\|y_2\|+\|y_3\|+\|y_4\|$ for all $y_1,y_2,y_3,y_4\in\mathbb{R}^d$, we obtain

$$\begin{aligned}&\left\|Y^{(n)}(t_{k+1}) - \frac{\theta}{\Gamma(\alpha)}\int_{t_k}^{t_{k+1}} \frac{f\left(t_{k+1}, Y^{(n)}(t_{k+1})\right) - f(t_{k+1},0)}{(t_{k+1}-s)^{1-\alpha}}\,ds\right\| \\ \le\ & \|y_0\| + \frac{\theta}{\Gamma(\alpha)}\int_{t_k}^{t_{k+1}} \frac{\|f(t_{k+1},0)\|}{(t_{k+1}-s)^{1-\alpha}}\,ds + \frac{\theta}{\Gamma(\alpha)}\int_0^{t_k} \frac{\|f(\lambda_n(s), Y^{(n)}(\lambda_n(s)))\|}{(t_{k+1}-s)^{1-\alpha}}\,ds \\ &+ \frac{(1-\theta)}{\Gamma(\alpha)}\int_0^{t_{k+1}} \frac{\|f(\zeta_n(s), Y^{(n)}(\zeta_n(s)))\|}{(t_{k+1}-s)^{1-\alpha}}\,ds.\end{aligned} \tag{14}$$

By directly using Assumption (H1) and condition (10), we arrive at

$$\begin{aligned}
&\left\| Y^{(n)}(t_{k+1}) - \frac{\theta}{\Gamma(\alpha)} \int_{t_k}^{t_{k+1}} \frac{f\left(t_{k+1}, Y^{(n)}(t_{k+1})\right) - f(t_{k+1}, 0)}{(t_{k+1}-s)^{1-\alpha}}\, ds \right\| \\
\geq\ & \|Y^{(n)}(t_{k+1})\| - \frac{\theta}{\Gamma(\alpha)} \int_{t_k}^{t_{k+1}} \frac{L_1 \|Y^{(n)}(t_{k+1})\|}{(t_{k+1}-s)^{1-\alpha}}\, ds \\
\geq\ & \|Y^{(n)}(t_{k+1})\| \left(1 - \frac{\theta\, L_1}{\Gamma(\alpha+1)} \left(\frac{T}{n}\right)^{\alpha}\right) \geq \frac{1}{2} \|Y^{(n)}(t_{k+1})\|.
\end{aligned}$$

Substituting this into (14), then apply the estimate (7) leads to

$$\begin{aligned}
\|Y^{(n)}(t_{k+1})\| \ \leq\ & 2\|y_0\| + \frac{2\,\theta\, M}{\Gamma(\alpha+1)} \left(\frac{T}{n}\right)^{\alpha} + \frac{2\,\theta\, M\, T^{\alpha}}{\Gamma(\alpha+1)} + \frac{2\,(1-\theta)\, M\, T^{\alpha}}{\Gamma(\alpha+1)} \\
+ & \frac{2\,\theta\, L_1}{\Gamma(\alpha)} \int_0^{t_k} \frac{\|Y^{(n)}(\lambda_n(s))\|}{(t_{k+1}-s)^{1-\alpha}} ds + \frac{2\,(1-\theta)\, L_1}{\Gamma(\alpha)} \int_0^{t_{k+1}} \frac{\|Y^{(n)}(\zeta_n(s))\|}{(t_{k+1}-s)^{1-\alpha}} ds. \qquad (15)
\end{aligned}$$

Next, to give an upper bound for $\sup_{0\leq t\leq T} \|Y^{(n)}(t)\|$, we need weight $E_\alpha(\mu\, t_{k+1}^{\alpha})$, where μ is a positive constant such that

$$\mu > 2L_1. \qquad (16)$$

From the increasing monotonicity of the functions $E_\alpha(\cdot)$ on $[0,\infty)$ and $f(s) = (t_{k+1}-s)^{\alpha-1}$, we have

$$\begin{aligned}
&\int_0^{t_k} \frac{\|Y^{(n)}(\lambda_n(s))\|}{(t_{k+1}-s)^{1-\alpha}\, E_\alpha(\mu\, t_{k+1}^{\alpha})}\, ds \\
\leq\ & \sum_{i=0}^{k-1} \int_{t_i}^{t_{i+1}} \frac{E_\alpha(\mu\, t_{i+1}^{\alpha})}{(t_{k+1}-s)^{1-\alpha} E_\alpha(\mu\, t_{k+1}^{\alpha})} \frac{\|Y^{(n)}(\lambda_n(s))\|}{E_\alpha(\mu\, (\lambda_n(s))^{\alpha})}\, ds \\
\leq\ & \sum_{i=0}^{k-1} \int_{t_{i+1}}^{t_{i+2}} \frac{E_\alpha(\mu\, s^{\alpha})}{(t_{k+1}-(s-\frac{T}{n}))^{1-\alpha} E_\alpha(\mu\, t_{k+1}^{\alpha})}\, ds \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^{\alpha})} \\
\leq\ & \int_0^{t_{k+1}} \frac{E_\alpha(\mu\, s^{\alpha})}{(t_{k+1}-s)^{1-\alpha} E_\alpha(\mu\, t_{k+1}^{\alpha})}\, ds \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^{\alpha})} \\
\leq\ & \frac{\Gamma(\alpha)}{\mu} \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^{\alpha})}, \qquad (17)
\end{aligned}$$

here in the final step, we used the following inequality

$$\frac{\mu}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} E_\alpha(\mu\, s^{\alpha})\, ds \leq E_\alpha(\mu\, t^{\alpha}),$$

see [13, Lemma 5].

Observing that $\zeta_n(s) \leq s$, hence in a similar manner as above, we get

$$\int_0^{t_{k+1}} \frac{\|Y^{(n)}(\zeta_n(s))\|}{(t_{k+1}-s)^{1-\alpha}\, E_\alpha(\mu\, t_{k+1}^\alpha)}\, ds \;\leq\; \frac{\Gamma(\alpha)}{\mu} \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^\alpha)}.$$

Inserting this and (17) into (15) leads to

$$\begin{aligned}
&\sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^\alpha)} \\
\leq\;& \frac{2\theta L_1}{\mu} \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^\alpha)} + \frac{2\,(1-\theta)\,L_1}{\mu} \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^\alpha)} + 2\|y_0\| + \frac{2M(1+\theta)\,T^\alpha}{\Gamma(\alpha+1)}.
\end{aligned}$$

Consequently,

$$\left(1 - \frac{2L_1}{\mu}\right) \sup_{0\leq t\leq T} \frac{\|Y^{(n)}(t)\|}{E_\alpha(\mu\, t^\alpha)} \;\leq\; 2\|y_0\| + \frac{2M(1+\theta)\,T^\alpha}{\Gamma(\alpha+1)}.$$

The condition (16) gives

$$\sup_{0\leq t\leq T} \|Y^{(n)}(t)\| \;\leq\; \left(2\|y_0\| + \frac{2M(1+\theta)\,T^\alpha}{\Gamma(\alpha+1)}\right) \frac{\mu\, E_\alpha\,(\mu\, T^\alpha)}{\mu - 2L1},$$

which completes the proof. □

Secondly, we determine an upper bound on $\|Y^{(n)}(t) - Y^{(n)}(t_1)\|$ in terms of $|t-t_1|^\alpha$.

Lemma 3.2. *Let*

$$C_2 := \frac{2(M + L_1 C_1)}{\Gamma(\alpha+1)}, \tag{18}$$

where C_1 is given as in (12)*. Then, for all $n \geq N$ and $t, t_1 \in [0,T]$,*

$$\|Y^{(n)}(t) - Y^{(n)}(t_1)\| \leq C_2 |t-t_1|^\alpha.$$

Proof. Choose and fix $t, t_1 \in [0,T]$ with $t > t_1$. From (5), we obtain

$$\begin{aligned}
&Y^{(n)}(t) - Y^{(n)}(t_1) \\
=\;& \frac{\theta}{\Gamma(\alpha)} \int_{t_1}^t \frac{f(\lambda_n(s), Y^{(n)}(\lambda_n(s)))}{(t-s)^{1-\alpha}} ds + \frac{(1-\theta)}{\Gamma(\alpha)} \int_{t_1}^t \frac{f(\zeta_n(s), Y^{(n)}(\zeta_n(s)))}{(t-s)^{1-\alpha}} ds \\
&+ \frac{\theta}{\Gamma(\alpha)} \int_0^{t_1} \Big(\frac{1}{(t-s)^{1-\alpha}} - \frac{1}{(t_1-s)^{1-\alpha}}\Big) f(\lambda_n(s), Y^{(n)}(\lambda_n(s)))\, ds \\
&+ \frac{(1-\theta)}{\Gamma(\alpha)} \int_0^{t_1} \Big(\frac{1}{(t-s)^{1-\alpha}} - \frac{1}{(t_1-s)^{1-\alpha}}\Big) f(\zeta_n(s), Y^{(n)}(\zeta_n(s)))\, ds.
\end{aligned}$$

Using the inequality $\|y_1 + y_2 + y_3 + y_4\| \le \|y_1\| + \|y_2\| + \|y_3\| + \|y_4\|$ for all $y_1, y_2, y_3, y_4 \in \mathbb{R}^d$, and by (7), we obtain

$$\begin{aligned}
&\left\|Y^{(n)}(t) - Y^{(n)}(t_1)\right\| \\
\le\ & \frac{\theta}{\Gamma(\alpha)} \int_{t_1}^{t} \frac{M + L_1 \|Y^{(n)}(\lambda_n(s))\|}{(t-s)^{1-\alpha}} ds + \frac{(1-\theta)}{\Gamma(\alpha)} \int_{t_1}^{t} \frac{M + L_1 \|Y^{(n)}(\zeta_n(s))\|}{(t-s)^{1-\alpha}} ds \\
&+ \frac{\theta}{\Gamma(\alpha)} \int_0^{t_1} \Big(\frac{1}{(t_1-s)^{1-\alpha}} - \frac{1}{(t-s)^{1-\alpha}} \Big) (M + L_1 \|Y^{(n)}(\lambda_n(s))\|)\, ds \\
&+ \frac{(1-\theta)}{\Gamma(\alpha)} \int_0^{t_1} \Big(\frac{1}{(t_1-s)^{1-\alpha}} - \frac{1}{(t-s)^{1-\alpha}} \Big) (M + L_1 \|Y^{(n)}(\zeta_n(s))\|)\, ds.
\end{aligned}$$

Using Lemma 3.1, we obtain

$$\begin{aligned}
&\left\|Y^{(n)}(t) - Y^{(n)}(t_1)\right\| \\
\le\ & \int_{t_1}^{t} \frac{M + L_1 C_1}{\Gamma(\alpha)\,(t-s)^{1-\alpha}} ds + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} \Big(\frac{1}{(t_1-s)^{1-\alpha}} - (t-s)^{1-\alpha} \Big) (M + L_1 C_1) ds.
\end{aligned}$$

A direct computation gives

$$\|Y^{(n)}(t) - Y^{(n)}(t_1)\| \le \frac{2(M + L_1 C_1)}{\Gamma(\alpha+1)} (t - t_1)^{\alpha},$$

which completes proof. □

We are now in a position to prove Theorem 2.1 (ii).

Proof of Theorem 2.1 (ii). Choose and fix $y_0 \in \mathbb{R}^d$. From (4) and (5) we receive

$$\begin{aligned}
Y^{(n)}(t) - Y(t) &= \frac{\theta}{\Gamma(\alpha)} \int_0^t \frac{f(\lambda_n(s), Y^{(n)}(\lambda_n(s))) - f(s, Y(s))}{(t-s)^{1-\alpha}}\, ds. \\
&\quad + \frac{1-\theta}{\Gamma(\alpha)} \int_0^t \frac{f(\zeta_n(s), Y^{(n)}(\zeta_n(s))) - f(s, Y(s))}{(t-s)^{1-\alpha}}\, ds.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\|Y^{(n)}(t) - Y(t)\| &= \frac{\theta}{\Gamma(\alpha)} \int_0^t \frac{\|f(\lambda_n(s), Y^{(n)}(\lambda_n(s))) - f(s, Y(s))\|}{(t-s)^{1-\alpha}}\, ds. \\
&\quad + \frac{1-\theta}{\Gamma(\alpha)} \int_0^t \frac{\|f(\zeta_n(s), Y^{(n)}(\zeta_n(s))) - f(s, Y(s))\|}{(t-s)^{1-\alpha}}\, ds. \qquad (19)
\end{aligned}$$

In view of Assumptions (H1) and (H2) it is easily seen that

$$\begin{aligned}
&\|f(\lambda_n(s), Y^{(n)}(\lambda_n(s))) - f(s, Y(s))\| \\
\le\ & L_1 \|Y^{(n)}(\lambda_n(s)) - Y(s)\| + L_2 |\lambda_n(s) - s|^{\beta}. \qquad (20)
\end{aligned}$$

By definition of ρ_n, we have $|\lambda_n(s)-s| \le \frac{T}{n}$ for $s \in [0,T]$. This together Lemma 3.2 implies that

$$
\begin{aligned}
&\|f(\lambda_n(s), Y^{(n)}(\lambda_n(s))) - f(s, Y(s))\| \\
&\le L_1 \, \|Y^{(n)}(\lambda_n(s)) - Y^{(n)}(s)\| + L_1 \, \|Y^{(n)}(s) - Y(s)\| + L_2 \left(\frac{T}{n}\right)^{\beta} \\
&\le L_1 \, C_2 \, |\lambda_n(s) - s|^{\alpha} + L_1 \, \|Y^{(n)}(s) - Y(s)\| + L_2 \left(\frac{T}{n}\right)^{\beta} \\
&\le L_1 \, C_2 \, T^{\alpha} \, \frac{1}{n^{\alpha}} + L_2 \, T^{\beta} \, \frac{1}{n^{\beta}} + L_1 \, \|Y^{(n)}(s) - Y(s)\|, \qquad (21)
\end{aligned}
$$

where C_2 is given as in (18).

Similarly, we have

$$
\|f(\zeta_n(s), Y^{(n)}(\zeta_n(s))) - f(s, Y(s))\| \le L_1 \, C_2 \, T^{\alpha} \, \frac{1}{n^{\alpha}} + L_2 \, T^{\beta} \, \frac{1}{n^{\beta}} + L_1 \, \|Y^{(n)}(s) - Y(s)\|.
$$

Injecting this, (20), and (21) into (19) results in

$$
\|Y^{(n)}(t) - Y(t)\| \le \frac{L_1}{\Gamma(\alpha)} \int_0^t \frac{\|Y^{(n)}(s) - Y(s)\|}{(t-s)^{1-\alpha}} \, ds + \frac{L_1 \, C_2 \, T^{2\alpha}}{\Gamma(\alpha+1)} \, \frac{1}{n^{\alpha}} + \frac{L_2 \, T^{\alpha+\beta}}{\Gamma(\alpha+1)} \, \frac{1}{n^{\beta}}.
$$

Applying the Gronwall inequality for FDEs (see e.g., [11, Lemma 6.19]), we obtain

$$
\|Y^{(n)}(t) - Y(t)\| \le \frac{(L_1 \, C_2 \, T^{2\alpha} + L_2 \, T^{\alpha+\beta}) E_{\alpha}(L_1 \, T^{\alpha})}{\Gamma(\alpha+1)} \, \frac{1}{n^{\kappa}}.
$$

With

$$
C := \frac{(L_1 \, C_2 \, T^{2\alpha} + L_2 \, T^{\alpha+\beta}) E_{\alpha}(L_1 \, T^{\alpha})}{\Gamma(\alpha+1)}
$$

this completes the proof of Theorem 2.1 (ii). □

4. A numerical example

We investigate numerically a simple Caputo FDEs for which we have an explicit expression for the solution. In particular, we consider a simple scalar linear Caputo FDEs

$$
{}^{C}D^{\alpha}_{0+} Y(t) = Y(t) \qquad (22)
$$

on interval $[0,1]$. It has the exact solution for $Y(0) = 1$ is given by $Y(1) = E_{\alpha}(1)$ (see e.g. [11, p. 135]). Moreover, $Y(1)$ has the integral representation

$$
Y(1) = 1 + \frac{1}{\Gamma(\alpha)} \int_0^1 \frac{Y(s)}{(1-s)^{1-\alpha}} \, ds.
$$

The convergence rates obtained are consistent with that stated in Theorem 2.1, which are for the whole class of vector fields and can be better in individual cases.

4.1. **Explicit case: $\theta = 0$.** The recursion expression (6) for the numerical solution simplifies to

$$Y_{k+1}^{(n)} = 1 + \sum_{j=0}^{k} \gamma_{k-j}\, Y_j^{(n)}\, \frac{1}{n^{\alpha}}, \qquad k = 0, \ldots, n-1.$$

Denote the global discretization error between the numerical solution $Y_n^{(n)}$ and the exact solution $Y(1)$ by

$$e_n = |Y(1) - Y_n^{(n)}| = |E_\alpha(1) - Y_n^{(n)}|$$

and the experimental order of convergence (EOC) by

$$\mathrm{EOC} := \log_2 \frac{\mathrm{e_n}}{\mathrm{e_{2n}}} = \log_2 \frac{|\mathrm{E}_\alpha(1) - \mathrm{Y_n^{(n)}}|}{|\mathrm{E}_\alpha(1) - \mathrm{Y_{2n}^{(2n)}}|},$$

see e.g. [17, p. 8].

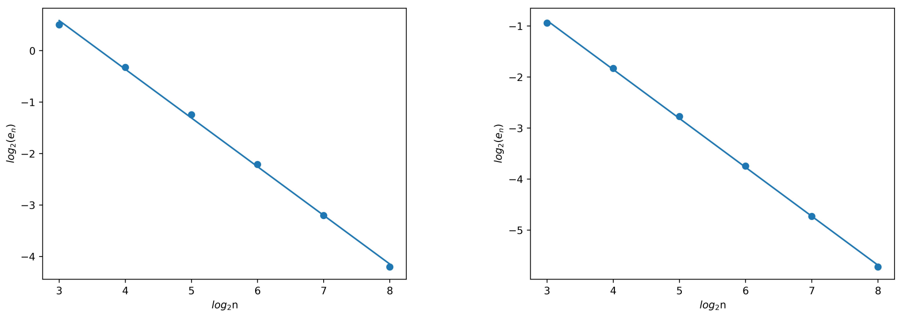
The results for the global discretization error, EOC and computational cost of the θ-scheme with $\theta = 0$ are given in the **Tab. 1**. All time values in the **Tab. 1** are given in seconds.

	$\alpha = 0.5$			$\alpha = 0.9$		
	e_n	EOC	Time	e_n	EOC	Time
$n = 8$	1.4158	0.8262	0.0010	0.5202	0.8880	0.0003
$n = 16$	0.7985	0.9186	0.0010	0.2811	0.9419	0.0000
$n = 32$	0.4224	0.9680	0.0040	0.1463	0.9706	0.0016
$n = 64$	0.2160	0.9912	0.0050	0.0747	0.9853	0.0037
$n = 128$	0.1086	1.0008	0.0160	0.0377	0.9928	0.0156
$n = 256$	0.0543	1.0041	0.0588	0.0190	0.9964	0.0568
$n = 512$	0.0271	1.0047	0.2218	0.0095	0.9982	0.2702

TABLE 1. Global error, EOC and computational cost for the θ-scheme with $\theta = 0$

The slopes of the lines in the coordinate system with the horizontal axis being $\log_2 n$ and the vertical axis being $\log_2(e_n)$ in **Fig. 1(a)** and **Fig. 1(b)** give the convergence rates of the θ-scheme with $\theta = 0$ for $\alpha = 0.5$ and $\alpha = 0.9$:

$$\alpha = 0.5 : \mathit{slope} = -0.9464465128045231, \quad \alpha = 0.9 : \mathit{slope} = -0.9587708473867738.$$



(A) $\alpha = 0.5$, slope = -0.9464465128045231

(B) $\alpha = 0.9$, slope = -0.9587708473867738

FIGURE 1. Convergence rate for the θ-scheme with $\theta = 0$.

4.2. **Implicit case** $\theta = 0.5$ **.** The recursion expression (6) simplifies to

$$Y_{k+1}^{(n)} = Y_0^{(n)} + \sum_{j=0}^{k} \gamma_{k-j} \left[(1-\theta)\, Y_j^{(n)} + \theta\, Y_{j+1}^{(n)}\right] \frac{1}{n^\alpha},$$

This is uniquely solvable for $n \geq \sqrt[\alpha]{\frac{2\,\theta}{\Gamma(\alpha+1)}}$ and is linear, so can be solved algebraically to give

$$Y_{k+1}^{(n)} = \Gamma_n\, Y_0^{(n)} + \gamma_0\, \Gamma_n\, (1-\theta)\, Y_k^{(n)} \frac{1}{n^\alpha} + \Gamma_n \sum_{j=0}^{k-1} \gamma_{k-j} \left[(1-\theta)\, Y_j^{(n)} + \theta\, Y_{j+1}^{(n)}\right] \frac{1}{n^\alpha}, \quad k = 0, \ldots, n-$$

where $\Gamma_n := \frac{1}{1-\gamma_0 \frac{1}{n^\alpha}}$.

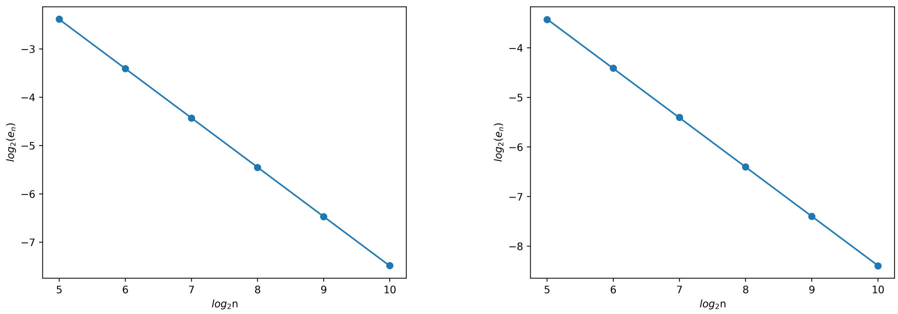
Results on the global discretization error, EOC and computational costs of the θ scheme with $\theta = 0.5$ are given in the **Tab. 2**.

	$\alpha = 0.5$			$\alpha = 0.9$		
	e_n	EOC	Time	e_n	EOC	Time
$n = 32$	0.1917	1.0234	0.0010	0.0928	0.9825	0.0010
$n = 64$	0.0943	1.0251	0.0066	0.0469	0.9913	0.0060
$n = 128$	0.0463	1.0221	0.0233	0.0236	0.9957	0.0215
$n = 256$	0.0228	1.0177	0.0884	0.0118	0.9979	0.0878
$n = 512$	0.0113	1.0136	0.3773	0.0059	0.9989	0.3826
$n = 1024$	0.0056	1.0102	1.4344	0.0030	0.9995	1.5066
$n = 2048$	0.0028	1.0075	5.9136	0.0015	0.9997	5.5054

TABLE 2. Global error, EOC and computational cost for θ-scheme with $\theta = 0.5$

The slopes of the lines in **Fig. 2(a)** and **Fig. 2(b)** give the convergence rates of the θ-scheme with $\theta = 0.5$ for $\alpha = 0.5$ and $\alpha = 0.9$.

$\alpha = 0.5$: *slope* $= -1.0207618200185753$, $\alpha = 0.9$: *slope* $= -0.9937723963388096$.



(A) $\alpha = 0.5$, slope = -1.0207618200185753 (B) $\alpha = 0.9$, slope = -0.9937723963388096.

FIGURE 2. Convergence rate for θ-scheme with $\theta = 0.5$.

4.3. **Fully implicit case $\theta = 1$.** For $n \geq \sqrt[\alpha]{\frac{2\,\theta}{\Gamma(\alpha+1)}}$ the θ-scheme (6) with $\theta = 1$ has a unique numerical solution $Y^{(n)}$ of

$$Y_{k+1}^{(n)} = Y_0^{(n)} + \sum_{j=0}^{k} \gamma_{k-j}\, Y_{j+1}^{(n)} \frac{1}{n^\alpha}, \qquad k = 0, \dots, n-1,$$

which is linear and thus can be solved algebraically to give

$$Y_{k+1}^{(n)} = \Gamma_n\, Y_0^{(n)} + \Gamma_n \sum_{j=0}^{k-1} \gamma_{k-j}\, Y_{j+1}^{(n)} \frac{1}{n^\alpha}, \qquad k = 0, \dots, n-1,$$

where $\Gamma_n := \frac{1}{1-\gamma_0 \frac{1}{n^\alpha}}$.

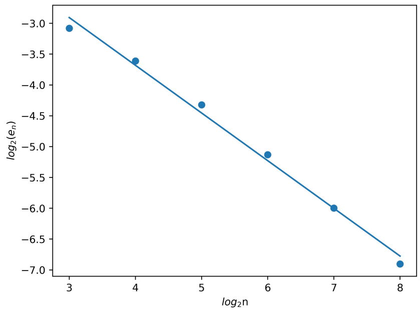
Results on the global discretization error, EOC and computational costs of the θ scheme with $\theta = 1$ are given in the **Tab. 3**.

	$\alpha = 0.5$			$\alpha = 0.9$		
	e_n	EOC	Time	e_n	EOC	Time
$n = 8$	0.1182	0.53023	0.0010	0.1589	1.0327	0.0010
$n = 16$	0.0819	0.7122	0.0010	0.0777	1.0188	0.0000
$n = 32$	0.0500	0.8076	0.0030	0.0383	1.0109	0.0010
$n = 64$	0.0285	0.8666	0.0120	0.0190	1.0063	0.0070
$n = 128$	0.0157	0.9062	0.0389	0.0095	1.0036	0.0259
$n = 256$	0.0084	0.9336	0.1606	0.0047	1.0021	0.0898
$n = 512$	0.0044	0.9529	0.6361	0.0024	1.0012	0.3405

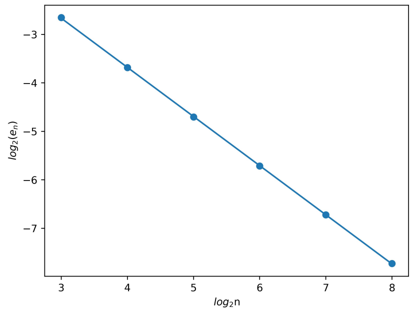
TABLE 3. Global error, EOC and computational cost for the θ-scheme with $\theta = 1$.

The slopes of the lines in **Fig. 3(a)** and **Fig. 3(b)** give the convergence rates of the θ-scheme with $\theta = 1$ for $\alpha = 0.5$ and $\alpha = 0.9$.

$$\alpha = 0.5 : slope = -0.7737488258780804, \quad \alpha = 0.9 : slope = -1.0136941007464315.$$



(A) $\alpha = 0.5$, slope = -0.7737488258780804



(B) $\alpha = 0.9$, slope = -1.0136941007464315.

FIGURE 3. Convergence rate for the θ-scheme with $\theta = 1$.

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