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2018

Li, X., & Wong, P. J. Y. (2018). High order approximation to new generalized Caputo fractional derivatives and its applications. AIP Conference Proceedings, 1978(1), 130006-. doi:10.1063/1.5043779

<https://hdl.handle.net/10356/88683>

<https://doi.org/10.1063/1.5043779>

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High Order Approximation to New Generalized Caputo Fractional Derivatives and its Applications

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Abstract. In this paper, we shall develop a generalized $L1 - 2$ formula for new generalized fractional Caputo derivatives. It is theoretically shown that this new approximation achieves $O(\tau^{3-\alpha})$ (τ is the step size) which improves earlier work done to date. Also, numerical tests and an application are presented to demonstrate the efficiency and accuracy of the proposed method.

INTRODUCTION

Fractional problems have been extensively investigated during past four decades since various phenomena are modeled more accurately using fractional operators [1, 2]. There are some existing analytical techniques developed in [1] for fractional models. However, it is extremely difficult to get explicit expression of solutions in most cases. Therefore, it is both necessary and meaningful to put efforts in studying numerical schemes.

In tackling fractional models numerically, an efficient and accurate approximation of fractional derivatives is essential. In general, for Caputo fractional derivatives ($0 < \alpha < 1$), $L1$ discretization [3] ($O(\tau^{2-\alpha})$), $L1 - 2$ formula [4] ($O(\tau^{3-\alpha})$), $O(\tau^{4-\alpha})$ method [5], $O(\tau^{r+1-\alpha})$ ($r \geq 4$) scheme [6], $L2 - 1_\sigma$ method [7] ($O(\tau^{3-\alpha})$) and weighted shifted Grünwald-Letnikov technique in [8] ($O(\tau^2)$) and [9] ($O(\tau^3)$) are applied successfully in various applications.

Recently, Agrawal [10] did a survey on some generalizations of fractional operators and then presented a **new** generalization involving a scale function $z(t)$ which allows one to stretch or contract the response domain, and a weight function $w(t)$ that can weigh differently at different time points. Thereafter this new generalized Caputo fractional operator has been applied to model various processes [11, 12, 13].

The main difficulty in deriving numerical scheme lies in the approximation of the generalized Caputo fractional derivative. In [11, 12, 13], they apply a useful approximation ($O(\tau^{2-\alpha})$) that generalizes the classical $L1$ discretization [3] in the sense that it coincides with $L1$ when $w(t) \equiv 1$ and $z(t) = t$. In this paper, we shall propose a high order approximation method which generalizes the classical $L1 - 2$ formula and investigate the efficiency of this approximation in an application.

HIGH ORDER APPROXIMATION

In this part, we shall derive a high order approximation for new generalized Caputo fractional derivative ($0 < \alpha < 1$) discussed in [10] with weight function $w(t) \equiv 1$. To begin, let us recall the definition of the generalized Caputo fractional derivative of a sufficiently smooth function $f(t)$ defined for $t \in [0, 1]$.

Definition 1. The generalized Caputo fractional derivative ($0 < \alpha < 1$) of $f(t)$ with respect to a weight function $w(t) \equiv 1$ and a scale function $z(t)$ is defined as $(D_{0,[z;1]}^\alpha f)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f'(s)}{[z(t)-z(s)]^\alpha} ds$.

Next, let $P : 0 = t_0 < t_1 < \dots < t_{N-1} < t_N = 1$ be the uniform partition of $[0, 1]$ with step size $\tau = \frac{1}{N}$ and $z(t)$ be a strictly increasing function. Also, for notational simplicity, we denote $f^n = f(t_n)$, $z^n = z(t_n)$ and $\delta_{t;[z;1]} f^{n+\frac{1}{2}} = (f^{n+1} - f^n)/(z^{n+1} - z^n)$.

Now, we are ready to develop the high order generalized $L1$ formula ($gL1 - 2$) for the generalized Caputo fractional derivative. First, we observe at $t = t_n$ that

$$D_{0;[z;1]}^\alpha f(t_n) = \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_1} [z^n - z(s)]^{-\alpha} f'(s) ds + \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} [z^n - z(s)]^{-\alpha} f'(s) ds \right]. \quad (1)$$

Next, we shall construct the linear interpolation of (z_0, f^0) and (z^1, f^1) by

$$\Pi_1 = \frac{z(t) - z^0}{z^1 - z^0} f^1 + \frac{z(t) - z^1}{z^0 - z^1} f^0,$$

and quadratic interpolation of (z^{k-1}, f^{k-1}) , (z^k, f^k) and (z^{k+1}, f^{k+1}) using

$$\Pi_k = \frac{(z(t) - z^k)(z(t) - z^{k+1})}{(z^{k-1} - z^k)(z^{k-1} - z^{k+1})} f^{k-1} + \frac{(z(t) - z^{k-1})(z(t) - z^{k+1})}{(z^k - z^{k-1})(z^k - z^{k+1})} f^k + \frac{(z(t) - z^{k-1})(z(t) - z^k)}{(z^{k+1} - z^{k-1})(z^{k+1} - z^k)} f^{k+1}, \quad k \geq 1. \quad (2)$$

Finally, using the linear interpolation to replace $f(t)|_{[t_0, t_1]}$ and the quadratic interpolation (2) to replace $f(t)|_{[t_k, t_{k+1}]}$ and then integrating, we shall obtain $gL1 - 2$ approximation

$$\bar{D}_{0;[z;1]}^\alpha f(t_n) = \frac{1}{\Gamma(2-\alpha)} \left[\sum_{k=0}^{n-1} a_k \delta_{t;[z;1]} f^{k+\frac{1}{2}} + \sum_{k=1}^{n-1} b_k \frac{\delta_{t;[z;1]} f^{k+\frac{1}{2}} - \delta_{t;[z;1]} f^{k-\frac{1}{2}}}{z^{k+1} - z^{k-1}} \right] = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} r_k \delta_{t;[z;1]} f^{k+\frac{1}{2}}, \quad (3)$$

where $a_k = (z^n - z^k)^{1-\alpha} - (z^n - z^{k+1})^{1-\alpha}$, $k \geq 0$ and $b_k = 2 \left[(z^n - z^k)^{2-\alpha} - (z^n - z^{k+1})^{2-\alpha} \right] / (2 - \alpha) - (z^{k+1} - z^k) \left[(z^n - z^k)^{1-\alpha} + (z^n - z^{k+1})^{1-\alpha} \right]$, $k \geq 1$ and $r_0 = a_0$ when $n = 1$ and if $n \geq 2$, then

$$r_k = \begin{cases} a_0 - \bar{b}_1, & k = 0, \\ a_k + \bar{b}_k - \bar{b}_{k+1}, & 1 \leq k \leq n-2, \\ a_{n-1} + \bar{b}_{n-1}, & k = n-1 \end{cases} \quad \text{where} \quad \bar{b}_k = \frac{b_k}{z^{k+1} - z^{k-1}}, \quad k \geq 1. \quad (4)$$

Now, following the procedure in Theorem 2.1 of [4], we shall get the accuracy of the approximation (3) which is illustrated by the theorem below.

Theorem 1. Assume that $Z : t \rightarrow z(t)$ is a bijection mapping function defined on $t \in [0, 1]$ and $\max_{0 \leq t \leq 1} |z'(t)| \leq C$. If $f(Z^{-1}(z)) = g(z) \in C^3[z(0), z(1)]$, we have $D_{0;[z;1]}^\alpha f(t_1) = \bar{D}_{0;[z;1]}^\alpha f(t_1) + O(\tau^{2-\alpha})$ and $D_{0;[z;1]}^\alpha f(t_n) = \bar{D}_{0;[z;1]}^\alpha f(t_n) + O(\tau^{3-\alpha})$, $n \geq 2$.

SIMULATION

In this section, we shall present some examples to verify the accuracy of this high order $gL1 - 2$ formula and to demonstrate the efficiency by tackling a new generalized fractional sub-diffusion problem [11].

Example 1. Let $z(t) = t^{\gamma_1}$ and $f(t) = t^{\gamma_2}$, then the generalized Caputo fractional derivative with $0 < \alpha < 1$ of function $f(t)$ is given by

$$(D_{0;[z;1]}^\alpha f)(t) = \left[\Gamma\left(\frac{\gamma_2}{\gamma_1} + 1\right) \right] \left[\Gamma\left(\frac{\gamma_2}{\gamma_1} + 1 - \alpha\right) \right] t^{\gamma_2 - \gamma_1 \alpha}.$$

To demonstrate the efficiency of $gL1 - 2$ formula numerically, we shall compare the performance of our $gL1 - 2$ formula with generalized $L1$ discretization ($gL1$) used in [11, 12, 13]. Table 1 presents the maximum absolute error at $t = 1$ and the convergence order for $\alpha = 0.2, 0.5$ and 0.8 of these two methods. Clearly, our method achieves $O(\tau^{3-\alpha})$ accuracy and gives the best result.

Next, we shall investigate the numerical treatment of the new generalized fractional sub-diffusion equation [11] using $gL1 - 2$ formula. The problem is stated as follows:

$$D_{0;[z;1]}^\alpha u(x, t) = \nu u_{xx}(x, t) + f(x, t), \quad x \in [0, L], \quad t \in [0, 1]$$

TABLE 1. (Example 1) Maximum absolute error at $t = 1$ and corresponding order when $\gamma_2 = 7.1$

$z(t) = t^{\gamma_1}$	τ	$\alpha = 0.2$	order	$\alpha = 0.5$	order	$\alpha = 0.8$	order
$\gamma_1 = 0.5$	$gL1[11]$	$\frac{1}{20}$	1.5955E-02	-	1.3698E-01	-	7.5679E-01
		$\frac{1}{40}$	5.2287E-03	1.6095	5.2578E-02	1.3814	3.4800E-01
		$\frac{1}{80}$	1.6571E-03	1.6578	1.9575E-02	1.4255	1.5602E-01
		$\frac{1}{160}$	5.1377E-04	1.6895	7.1560E-03	1.4518	6.9011E-02
$\gamma_1 = 0.5$	$gL1 - 2$	$\frac{1}{20}$	2.5903E-03	-	2.3160E-02	-	1.3527E-01
		$\frac{1}{40}$	4.3670E-04	2.5684	4.5930E-03	2.3341	3.2322E-02
		$\frac{1}{80}$	6.9870E-05	2.6439	8.6685E-04	2.4056	7.3804E-03
		$\frac{1}{160}$	1.0843E-05	2.6879	1.5926E-04	2.4444	1.6466E-03
$\gamma_1 = 1$	$gL1 [11]$	$\frac{1}{20}$	1.2761E-02	-	8.9492E-02	-	4.0286E-01
		$\frac{1}{40}$	4.1861E-03	1.6081	3.4342E-02	1.3818	1.8499E-01
		$\frac{1}{80}$	1.3278E-03	1.6566	1.2785E-02	1.4255	8.2879E-02
		$\frac{1}{160}$	4.1195E-04	1.6885	4.6742E-03	1.4517	3.6646E-02
$\gamma_1 = 1$	$gL1 - 2$	$\frac{1}{20}$	1.7525E-03	-	1.2813E-02	-	6.1027E-02
		$\frac{1}{40}$	2.9399E-04	2.5756	2.5243E-03	2.3436	1.4464E-02
		$\frac{1}{80}$	4.6935E-05	2.6470	4.7488E-04	2.4102	3.2891E-03
		$\frac{1}{160}$	7.2782E-06	2.6890	8.7112E-05	2.4466	7.3228E-04
$\gamma_1 = 2$	$gL1 [11]$	$\frac{1}{20}$	9.1795E-03	-	5.2869E-02	-	1.9453E-01
		$\frac{1}{40}$	3.0171E-03	1.6053	2.0277E-02	1.3826	8.9075E-02
		$\frac{1}{80}$	9.5855E-04	1.6542	7.5487E-03	1.4256	3.9851E-02
		$\frac{1}{160}$	2.9780E-04	1.6865	2.7603E-03	1.4514	1.7608E-02
$\gamma_1 = 2$	$gL1 - 2$	$\frac{1}{20}$	7.8452E-04	-	4.7197E-03	-	1.8406E-02
		$\frac{1}{40}$	1.3030E-04	2.5900	9.1768E-04	2.3626	4.2921E-03
		$\frac{1}{80}$	2.0710E-05	2.6534	1.7153E-04	2.4195	9.6799E-04
		$\frac{1}{160}$	3.2063E-06	2.6913	3.1370E-05	2.4510	2.1462E-04

with initial condition $u(x, 0) = u_0(x)$ and boundary conditions $u(0, t) = g_1(t)$, $u(L, t) = g_2(t)$.

Let $P' : 0 = x_0 < \dots < x_m < \dots < x_M = L$ be the uniform partition of $[0, L]$ with step size $h = \frac{L}{M}$. Discretizing above problem at (x_m, t_n) and applying $gL1 - 2$ formula coupled with finite difference method yield the numerical scheme

$$\frac{1}{\Gamma(2 - \alpha)} \sum_{k=0}^{n-1} r_k \delta_{t;[z;1]} u_m^{k+\frac{1}{2}} = v \delta_x^2 u_m^n + f_m^n \quad (5)$$

with conditions $u_m^0 = u_0(x_m)$ and $u_0^n = g_1(t_n)$, $u_M^n = g_2(t_n)$.

Example 2. [11] Let $\alpha = 0.85$, $v = L = 1$, $u(x, 0) = \sin(\pi x)$, $g_1(t) = g_2(t) = 0$ and $f(x, t) = \frac{2}{\Gamma(2.15)}(x^2 - x)t^{1.15} + \pi^2 \sin(\pi x) - 2t^2$. When $z(t) = t$, the exact solution of this problem is $u(x, t) = \sin(\pi x) + x(x - 1)t^2$.

Let $h = \frac{1}{512}$ and τ vary, in Table 2, we present the maximum absolute error and the temporal convergence order for $z(t) = t^{0.5}$, t , $t^{1.5}$ using $gL1 - 2$ approximation as well as for $z(t) = t$ using $gL1 [11]$. It is obvious that our method converges faster than $gL1$ and gives the smallest error as well. For visualization, in Figure 1, we plot the exact solution for $z(t) = t$ and numerical solutions obtained from (5) for $z(t) = t^{0.5}$, t , $t^{1.5}$ when $\tau = h = 0.01$.

CONCLUSION

In this paper, we propose a high order accuracy approximation method for the new generalized Caputo fractional derivative. The order of convergence of this method is established rigorously and it is shown that this approximation improves the generalized $L1$ discretization. To demonstrate the efficiency, we carry out a numerical test and an experi-

TABLE 2. (Example 2) Maximum absolute error and temporal convergence order for various scale function $z(t)$ when $h = \frac{1}{512}$

τ	$gL1 - 2$ formula						$gL1$ [11]	
	$z(t) = t^{0.5}$	order	$z(t) = t$	order	$z(t) = t^{1.5}$	order	$z(t) = t$	order
$\frac{1}{8}$	4.7967E-04		8.0485E-06		7.9732E-05		6.9354E-02	
$\frac{1}{16}$	1.0590E-04	2.1794	1.6880E-06	2.2534	1.6886E-05	2.2393	3.2568E-02	1.0905
$\frac{1}{32}$	2.3926E-05	2.1460	3.5201E-07	2.2616	3.6892E-06	2.1945	1.5781E-02	1.0453
$\frac{1}{64}$	5.4957E-06	2.1222	7.6472E-08	2.2026	8.1817E-07	2.1728	7.7736E-03	1.0215

FIGURE 1. (Example 2) Exact (top, left) and numerical (top, right) solutions for $z(t) = t$; numerical solutions for $z(t) = t^{0.5}$ (bottom, left) and $z(t) = t^{1.5}$ (bottom, right).

ment in application. Both cases indicate this $gL1 - 2$ formula can achieve high accuracy and perform better than some earlier work.

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