A numerical evaluation and regularization of Caputo fractional derivatives

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Abstract. Numerical evaluations of Caputo fractional derivatives for scattered noisy data is an important problem in scientific research and practical applications. Fractional derivatives have been applied recently to the numerical solution of problems in fluid and continuum mechanics. The Caputo fractional derivative of order \(\alpha\) is given as follows:

\[ f^{(\alpha)}(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f^{(n)}(s)}{(t-s)^\alpha} ds, \quad 0 < \alpha < 1 \]

The above definition includes a Volterra integral equation with weakly singular kernels and difficult to calculate. In this paper, a faster convergence numerical schedule is given and applied to solve several fractional-diffusion heat conduction problems. Convergence rates of interest are also presented here. Several numerical results are given to show the effectiveness of the proposed numerical schedule.

Keywords: Numerical derivatives; fractional derivatives; ill-posed; regularization

1. Introduction

Fractional derivatives have been applied recently in fluid and continuum mechanics. Numerical derivative is a typical ill-posed in the sense that a small error in measurement data can induce a large error in the approximate derivatives and important in science and engineering [8, 9]. With the recent successful application of fractional derivatives in mechanics problems, an accurate numerical evaluation of fractional derivatives from scattered noisy data is important in scientific research and practical industries. Due to the ill-posedness of the numerical fractional derivative, both the convergence and stability of the numerical should be investigated.

In mathematics, the RiemannLiouville integral is defined by

\[ J^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (s-t)^{\alpha-1} f(s) ds \]  

(1)

Based on the the RiemannLiouville integral, the Caputo fractional derivative was introduced by Caputo in 1967:

\[ D^\alpha f(t) = J^{(n-\alpha)} D^n f(t), \quad n = \lceil \alpha \rceil \]  

(2)
where $\Gamma(\cdot)$ is the Gramma function. A number of computational methods have been researched in the past years: difference methods [2], Tikhonov regularization methods [3, 4], mollification methods [6, 7], fourier truncation method [1] and interpolation methods [5]. Most of these researches on numerical derivative are related to integer order derivative.

Although many numerical schemes are use to obtain the fractional order derivative, the difference method is still a simple and effective numerical method in one-dimensional case. In the present paper, we also give a new regularization difference method. Theoretical convergence and stability results and numerical examples will proposed and show the proposed regularization difference method is accurate and stable.

The structure of the paper is as follows. In Section 2, we briefly formulate the problem and propose the difference scheme. In Section 3, theoretical convergence and stability results are obtained respectively. In Section 4, numerical results illustrate the stability and accuracy of the proposed method.

2. Numerical Scheme

In this paper, let $\alpha \in (0, 1)$ and $n$ is a positive number. Let $f = f(x)$ be a function in $\mathbb{R}$ and $\{x_i = \frac{(b-a)i}{n}\}_{i=0}^n$ be a set of distinct points on $[a,b]$. Here, we consider the following problem: given the noisy measurement $\tilde{f}_i$ of the values $f(x_i)$ which satisfies

$$|\tilde{f}_i - f(x_i)| \leq \delta$$

where $\delta$ is called the noise level. The purpose of this paper is to obtain an approximate value of the Caputo derivative:

$$D_\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t f'(s)(t-s)^{\alpha-1}ds, \quad 0 < \alpha < 1$$

A difference scheme of Caputo fractional derivative

$$D^\alpha_k f(t_i) = \sigma_{\alpha,k} \sum_{j=0}^i \omega_j f_j$$

where

$$\begin{align*}
\omega_0 &= (i-1)^{1-\alpha} - i^{1-\alpha} \\
\omega_j &= (i-j+1)^{1-\alpha} - 2(i-j)^{1-\alpha} + (i-j-1)^{1-\alpha} \\
\omega_i &= 1 \\
\sigma_{\alpha,k} &= \frac{1}{\Gamma(1-\alpha)} \frac{1}{(1-\alpha)k^{\alpha}}
\end{align*}$$

3. Error Estimate

**Lemma 3.1** Suppose that $\| f \|_\infty \leq E$. For any $t \in (t_i - \frac{k}{2}, t_i + \frac{k}{2}]$, $D^\alpha_k f(t) = D^\alpha_k f(t_i)$ which defined by the formula (5). Then

$$\| D^\alpha f(t) - D^\alpha_k f(t) \|_\infty \leq C k^{2-\alpha}$$

where $C$ is constants depending on $\alpha$ and $\| f''(t) \|_\infty$
Proof: First of all, we divide the integral (4) into two parts,

\[ D^\alpha f(t_i) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_i} \frac{f'(s)}{(t-s)^\alpha} ds \]

\[ = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_i-1} \frac{f'(s)}{(t-s)^\alpha} ds + \frac{1}{\Gamma(1-\alpha)} \int_{t_i-1}^{t_i} \frac{f'(s)}{(t-s)^\alpha} ds \]

(8) (9)

It’s obvious that I part is a normal integral without singularity. Using the integration by parts, we obtain

\[ I = f(s)(t_i - s)^{-\alpha}|_0^{t_i-1} - \alpha \int_0^{t_i-1} f(s)(t_i - s)^{-\alpha-1} ds \]

\[ = f_{i-1}k^{-\alpha} - f_0t_i^{-\alpha} - \alpha \sum_{j=1}^{i-1} \frac{f_{j-1} + f_j}{t_j-1} \]

\[ + f''(\xi_k)k^2(t_i - s)^{-\alpha-1} ds \]

(10) (11) (12)

And

\[ II = \int_{t_i-1}^{t_i} \left( \frac{f_i - f_{i-1}}{k} + kf''(\xi_k) \right) (t_i - s)^{-\alpha} ds \]

\[ = \frac{f_i - f_{i-1}}{(1-\alpha)k^\alpha} + f''(\xi_k)k^{2-\alpha} \]

(13) (14)

Substituting (13) and (14) into (4), we have

\[ D^\alpha f(t) = D^\alpha_k f(t_i) - \alpha \sum_{j=1}^{i-1} \int_{t_{j-1}}^{t_j} f''(\xi_k)k^2(t_i - s)^{-\alpha-1} ds + f''(\xi_k)k^{2-\alpha} \]

(15)

Therefore,

\[ \| D^\alpha f(t) - D^\alpha_k f(t) \|_\infty \leq \frac{\alpha + 1}{\Gamma(1-\alpha)} \| f'' \|_\infty k^{2-\alpha} \]

(16)

Lemma 3.2 Let \( D^\alpha_k \tilde{f}_i = \sigma_{\alpha,k} \sum_{j=0}^{i'} \omega_j \tilde{f}_j \). Then

\[ |D^\alpha_k f(t_i) - D^\alpha_k \tilde{f}_i| \leq \frac{\delta}{\Gamma(1-\alpha)(1-\alpha)k} \]

(17)
Proof: It’s not difficult to show that
\[
| D^\alpha_k f(t_i) - D^\alpha_k \tilde{f}_i | = \sigma_{\alpha,k} \sum_{j=0}^{i} \omega_j | f(t_j) - \tilde{f}_j | 
\]
(18)
\[
\leq \sigma_{\alpha,k} \delta \sum_{j=0}^{i} \omega_j \leq \frac{\delta n^{1-\alpha}}{\Gamma(1-\alpha)(1-\alpha)k^\alpha} 
\]
(19)
\[
= \frac{\Gamma(1-\alpha)(1-\alpha)}{\Gamma(1-\alpha)(1-\alpha)k} 
\]
(20)

As \( k \) tend to zero, the estimation of convergence (7) tent to zero. However, at the same time, the error (17) tent to infinity when the noise level \( \delta > 0 \). Hence, for balance them, the step size \( k \) should be chosen depending on the noise level \( \delta \). Then, combining the Lemma 1 and 2, the following theorem can be obtain.

**Theorem 3.3** Let \( k = \left( \frac{\delta}{(1-\alpha)^{\| f' \|_\infty}} \right)^{\frac{1}{1-\alpha}} \). Then
\[
\| D^\alpha f(t) - D^\alpha_k \tilde{f}_i \|_\infty \leq C' k^{\frac{2-\alpha}{1-\alpha}} 
\]
(21)
where \( C' = \left( \frac{(\alpha+1)^{\| f'' \|_\infty}}{(1-\alpha)^{1-\alpha}} \right)^{\frac{1}{1-\alpha}} \)

**Remark 3.4** In the real application, \( \| f'' \|_\infty \) is usually not known, therefore we have no the exact step size \( k(\delta) \). However, if we select \( k(\delta) = \left( \frac{\delta}{(1-\alpha)^{\| f' \|_\infty}} \right)^{\frac{1}{1-\alpha}} \), we can also obtain
\[
\| D^\alpha f(t) - D^\alpha_k \tilde{f}_i \|_\infty \leq C'' k^{\frac{2-\alpha}{1-\alpha}} 
\]
(22)
where the constant \( C'' \) just only depends on \( k \) and \( \| f'' \|_\infty \). The following numerical results show this choosing rule is still stable in the realistic computation.

**4. Numerical Examples**

To demonstrate the effectiveness and stability of the proposed difference method, the following example is presented in this section. For simplicity, we assume that the interval \([a, b]\) always be \([0, 1]\). The accuracy of the numerical solution is measured by the the following root mean square error (RMSE):
\[
RMSE = \sqrt{\frac{1}{n+1} \sum_{i=0}^{n} (D^\alpha f(t_i) - D^\alpha_k \tilde{f}_i)^2} 
\]
(23)

We consider a smooth function
\[
f(t) = t^2
\]
The exact \( \alpha \) order fractional derivative is
\[
D^\alpha f(t) = \frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha} 
\]
(24)
Figure 1 shows the exact α order fractional derivative with different parameter α. For illustrate the convergence of the proposed difference method, first of all, we compute the fractional derivatives without noise by using the formula (5). From Figure 2, it’s easy to see that the RMSEs by using our proposed algorithm converge to zero fast. And the numerical accuracies with small α are higher than large α. This is consistent with the theoretical result in Lemma 1.

![Figure 1](image1.png)

**Figure 1.** The exact α order fractional derivative with different parameter α.

![Figure 2](image2.png)

**Figure 2.** The RMSEs without noise for different numbers of points n

Then, for overcoming the ill-posedness, we choose the step size with the proposed rule \( k = \left( \frac{\delta}{1-\alpha^2} \right)^{1/\alpha} \). Figure 3 shows that the proposed regularization difference method is stable for solving the numerical fractional derivative with \( \alpha \in (0, 1) \).

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6. Conclusion

In this paper, a regularization difference method is proposed to solve numerical fractional derivatives. The convergence rate and the error estimation of the proposed method are obtained. Numerical results indicate that the proposed method gives an accurate and reliable scheme and performances.

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