Computational Algorithm for Approximating Fractional Derivatives of Functions

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ABSTRACT

This paper presents an algorithmic approach for numerically solving Caputo fractional differentiation. The trapezoidal rule was modified, the new modification was used to derive an algorithm to approximate fractional derivatives of order \( \alpha > 0 \), the fractional derivative used was based on Caputo definition for a given function by a weighted sum of function and its ordinary derivatives values at specified points. The trapezoidal rule was used in conjunction with the finite difference scheme which is the forward, backward and central difference to derive the computational algorithm for the numerical approximation of Caputo fractional derivative for evaluating functions of fractional order. The study was conducted through some illustrative examples and analysis of error.

Keywords: Fractional Calculus; Finite difference Scheme; Modified trapezoidal rule.

1 Introduction

Gottfried Wilhelm Leibniz traded ideas on fractional calculus (FC) with other mathematicians in 1695 which name “fractional calculus” were retained for historical reasons [1]. Until the past few decades when the research community began to notice its elegant and excellent performance for describing a wide range of artificial and natural processes which the integer–order was limited in, this scientific tool was mostly used in the field of pure mathematics [1], [2]. For a thorough examination of current advancement and understanding in FC the readers are directed for numerical analysis to [3]–[6] for physics to [7], [8] for economics to [9] for mathematics to [10]–[18] and for applications [1], [7]–[9], [13], [19]. Therefore, identifying not only obstacles, but potentials and also indicating a route for the future could have a big impact, as a result numerous strategies and tactics have been put forth [15], [20]–[37]. Recent study on this approach can be found, for example, in [38]–[43]. This article shares the author’s perspective on the major, and rapidly developing topic of fractional calculus and propose and algorithm for easy computation of functions with the aid of finite difference scheme and the trapezoidal rule, with this method the problems are resolved due to the methods high adaptability and applications are made easier while maintaining efficiency. Engineers and scientists use numerical integration which is fundamental to obtain approximations of definite integrals that are difficult to solve analytically [42], [43]. One method among others that can be used for approximation of definite integrals of a specific function value at particular points is the trapezoidal rule which is based on dividing the area between the curve of \( f(x) \) and the horizontal axis into strips and then interpolating the function \( f(x) \) by a sequence of (straight) lines [5]. Given that the interval \([a,b]\) is subdivided into \( M \) subintervals \([x_k,x_{k+1}]\) of width \( h = \frac{(b-a)}{M} \) by using the equally spaced nodes \( x_k = a + kh \) for \( k = 0, 1, ..., M \). The composite trapezoidal rule for \( M \) subintervals can be defined as [5], [6] and expressed in any of three equivalent ways:
\( T(f, h) = \frac{h}{2} \sum_{k=1}^{M} (f(x_{k-1}) + f(x_k)) \) \hspace{1cm} (1.0)

or

\( T(f, h) = \frac{h}{2} (f_0 + 2f_1 + 2f_2 + 2f_3 + \ldots + 2f_{m-2} + 2f_{m-1} + f_m) \) \hspace{1cm} (1.1)

or

\( T(f, h) = \frac{h}{2} (f(a) + f(b)) + h \sum_{k=1}^{M-1} f(x_k). \) \hspace{1cm} (1.2)

Which is an approximation of the integral of \( f(x) \) over \([a, b]\),

\( \int_a^b f(x) \, dx \approx T(f, h). \) \hspace{1cm} (1.3)

**Error Analysis**

If \( f(x) \in C^2 [x, y] \), then there is a value \( \tau \) with \( x < \tau < y \) so that the error term \( E(f, h) \) has the form

\[ E(f, h) = \frac{-(y-x)f^{(2)}(\tau)(h^2)}{12} = O(h^2) \] \hspace{1cm} (1.4)

and

\[ E(f, h) = \int_a^b f(x) \, dx - T(f, h). \] \hspace{1cm} (1.5)

**2 Materials and Techniques**

This section presents some Mathematical basics which will be necessary for further evaluation in this paper, some of which include definitions, properties and theorems and can be found in [5], [6], [42]–[44].

**2.1 The Caputo Fractional Derivative**

Given that \( m \) is the smallest integer greater than \( \alpha \), then Caputo fractional derivative of order \( \alpha > 0 \) is defined as [44]

\[ D^\alpha_x f(x) = f^{m-\alpha} f^m(x) \quad \text{with} \quad m - 1 < \alpha < m, \]

\[ D^\alpha_x f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \left[ \int_0^t \frac{f^{(m)}(\tau)}{(x-\tau)^{\alpha+1-m}} \, d\tau \right], & m - 1 < \alpha < m, \\ \frac{d^m}{dx^m} f(x), & \alpha = m. \end{cases} \] \hspace{1cm} (1.6)

For \( 0 < \alpha < 1 \), the true value of the fractional derivative \( D^\alpha_x \cos(x) \) is given by

\[ D^\alpha_x \cos(x) = x^{m-\alpha} \sum_{k=0}^{\infty} \frac{(-1)^k}{\Gamma(m-\alpha+2k+1)} x^{2k}. \] \hspace{1cm} (1.7)

**2.2 Modification of Trapezoidal Rule**

**Theorem 1**: Given that the interval \([0, a]\) is subdivided into \( k \) subintervals \([x_i, x_{i+1}]\) of equal width \( h = a/k \) by using the nodes \( x_j = jh \), for \( j = 0, 1, \ldots, k \) The modified trapezoidal rule is given as [43]

\[ T(f, h, \alpha) = ((k-1)x^{s+1} - (k - \alpha - 1) k^s) \frac{h^\alpha f(0)}{\Gamma(\alpha + 2)} + \frac{h^\alpha f(a)}{\Gamma(\alpha + 2)} \]

\[ + \sum_{j=1}^{k-1} (((k-j+1)x^{s+1} - 2k(j-1)x^{s+1} + (k-j-1)x^{s+1}) h^\alpha f(x_j)) \frac{h^\alpha f(x_j)}{\Gamma(\alpha + 2)}. \] \hspace{1cm} (1.8)

This is an approximation to fractional integral

\[ (I^\alpha f(x))(a) = T(f, h, \alpha) - E_T(f, h, \alpha), \quad \alpha > 0, \quad \alpha > 0. \] \hspace{1cm} (1.9)
Proof: From the Riemann–Liouville fractional integral operator $I^{\alpha}f(x)$ of order $\alpha > 0$ on the usual Lebesgue space $L_1[a, b]$ we have

$$I^{\alpha}(a) = \frac{1}{\Gamma(a)} \int_{0}^{a} (a - \tau)^{a-1} f(\tau) \, d\tau.$$  \hspace{1cm} (2.0)

If $f_k$ is the linear interpolant that is piecewise for $f$ whose nodes are chosen at $x_j, j = 0, 1, 2, \ldots, k$, then, we have

$$\int_{0}^{a} (a - \tau)^{a-1} f_k(\tau) \, d\tau = \frac{h^a}{a(a+1)} \left\{ (k - 1)^{\alpha+1} - (k - \alpha - 1)k^a \right\} f(0) + f(a) + \sum_{j=1}^{k} ((k - j + 1)^{\alpha+1} - 2(k - j)^{\alpha+1} + (k - j - 1)^{\alpha+1}) f(x_j) \right\} \leq C \|f''\|_\infty a^a h^2.$$

(2.1)

and

$$\left| \int_{0}^{a} (a - \tau)^{a-1} f(\tau) - \int_{0}^{a} (a - \tau)^{a-1} f_k(\tau) \, d\tau \right| \leq C_\alpha' \|f''\|_\infty a^a h^2.$$  \hspace{1cm} (2.2)

Thereafter theorem 1 from (2.1) and (2.2) where $C_\alpha' = C_\alpha / \Gamma(a)$.

This method behaves in a manner that is similar to the classical trapezoidal rule. Substituting $\alpha = 1$ the modified trapezoidal rule reduces to the classical trapezoidal rule.

2.3 Caputo Fractional Derivative Rule

Theorem 2: Suppose that the interval $[0, a]$ is subdivided in to $k$ subintervals $[x_j, x_{j+1}]$ of equal width $h = a/k$ by using the nodes $x_j = jh$, for $j = 0, 1, \ldots, k - 1$. Then we have the rule [43]

$$C(f, h, \alpha) = \frac{h^{m-a}}{\Gamma(m+2-\alpha)} \left\{ ((k - 1)^{m-\alpha+1} - (k - m + \alpha - 1)k^{m-\alpha}) f^{(m)}(0) + f^{(m)}(a) + \sum_{j=1}^{k} ((k - j)^{m-\alpha+1} - 2(k - j)^{m-\alpha+1} + (k - j - 1)^{m-\alpha+1}) f^{(m)}(x_j) \right\},$$

(2.3)

This gives an approximation to the fractional derivative by Caputo

$$(D^\alpha f(x))(a) = C(f, h, \alpha) - E_T(f, h, \alpha), \: \alpha > 0, m - 1 < \alpha \leq m$$

(2.4)

Furthermore, if $f(x) \in C^{m+1}[0, a]$ then there is a constant $C'_\alpha$ depending strictly on $\alpha$ so that the error term $E_C(f, h, \alpha)$ is expressed as

$$|E_C(f, h, \alpha)| \leq C'_\alpha \|f^{(m+2)}\|_\infty a^{m-\alpha} h^2 = O(h^2).$$

(2.5)

If we replace the term $f^{(m)}(x_j), m - 1 < \alpha \leq m$, on the right-hand side of (2.3) with the required formula from the finite difference formulas [5], [6] and by cancelling the term $h^m$, we obtain the general term

$$(D^\alpha f)(x) = \frac{h^{-\alpha}}{\Gamma(m+2-\alpha)} \left\{ \sum_{j=1}^{k} ((k - j + 1)^{m-\alpha+1} - 2(k - j)^{m-\alpha+1} + (k - j - 1)^{m-\alpha+1}) g_m(x_j) + g_m(a) \right\} + E(f, h, \alpha), \: m - 1 < \alpha \leq m.$$  \hspace{1cm} (2.6)

In the case of $0 < \alpha < 1$, then the Caputo fractional derivative rule (2.3) diminishes to the formula

$$C(f, h, \alpha) = \frac{h^{-1-\alpha}}{\Gamma(3-\alpha)} \left\{ \sum_{j=1}^{k} ((k - j + 1)^{2-\alpha} - 2(k - j)^{2-\alpha} + (k - j - 1)^{2-\alpha}) f^{(3)}(x_j) \right\},$$

(2.7)

If $f(x) \in C^3[0, a]$ error term $E_C(f, h, \alpha)$ is given as

$$|E_C(f, h, \alpha)| \leq C'_1 \|f^{(3)}\|_\infty \alpha^{1-\alpha} h^2 = O(h^2).$$

(2.8)

For some constant $C'_1$ depending strictly on $\alpha$
Proof: Considering definition (1.6), replace $\alpha$ by $m - \alpha$ and $f(x_j)$ by $f^{(m)}(x_j)$ in Theorem 1.

Where $f^{(m)}(x_j)$ is the forward, backward or central difference formulas to the $m^{th}$ derivatives as well as many other finite difference formulas for approximating derivatives, can be derived by using Taylor’s series expansion [5], [6].

When $1 < \alpha < 2$, the Caputo fractional derivative rule (2.3) minimizes to the formula

$$C(f, h, \alpha) = \frac{h^{2-\alpha}}{\Gamma(4-\alpha)} \left\{ \frac{((k - 1)^{3-\alpha} - (k + \alpha - 3)k^{2-\alpha})f''(0) + f''(a)}{3!} + \sum_{j=1}^{\infty} \frac{(k - j + 1)^{3-\alpha} - 2(k - j)^{3-\alpha} + (k - j - 1)^{3-\alpha})f''(x_j)}{\alpha} \right\}$$

(2.9)

If $f(x) \in C^4[0, a]$ error term $E_C(f, h, \alpha)$ is given as

$$|E_C(f, h, \alpha)| \leq C_{2-\alpha}'f^{(4)}\|\alpha^2\alpha h^2 = 0(h^2).$$

(3.0)

For some constant $C_{2-\alpha}'$ depending strictly on $\alpha$

3 Theory/Calculation

We shall consider here some problems of interest for the illustration of the method of the preceding section.

The concept offered above are closely followed in this section, we limit ourselves to the instance of $0 < \alpha < 1$ for the purpose of conciseness. It is to be noted that the results presented in the tables below were obtained using MATLAB 2016a package.

Example 1: Consider the function $f(x) = \cos x$, in Tables 1-3 using the definition of Caputo fractional derivative.

Table 1: The approximate value for the Caputo fractional derivative rule using the central formula: $D^{0.75}_0\cos (x)$(1)

<table>
<thead>
<tr>
<th>$K$</th>
<th>$h$</th>
<th>$T(f, h, 0.75)$</th>
<th>$T_T(f, h, 0.75)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1</td>
<td>-0.765492171</td>
<td>0.001710770</td>
</tr>
<tr>
<td>20</td>
<td>0.05</td>
<td>-0.766766373</td>
<td>0.000436305</td>
</tr>
<tr>
<td>40</td>
<td>0.025</td>
<td>-0.767092116</td>
<td>0.000110825</td>
</tr>
<tr>
<td>80</td>
<td>0.0125</td>
<td>-0.767174873</td>
<td>0.000028069</td>
</tr>
<tr>
<td>160</td>
<td>0.00625</td>
<td>-0.767195848</td>
<td>0.000007093</td>
</tr>
<tr>
<td>320</td>
<td>0.003125</td>
<td>-0.767201152</td>
<td>0.000001789</td>
</tr>
</tbody>
</table>

Table 2: The approximate value for the Caputo fractional derivative rule using the forward difference formula: $D^{0.75}_0\cos (x)$(1)

<table>
<thead>
<tr>
<th>$K$</th>
<th>$h$</th>
<th>$T(f, h, 0.75)$</th>
<th>$T_T(f, h, 0.75)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1</td>
<td>-0.769500650</td>
<td>0.00297702</td>
</tr>
<tr>
<td>20</td>
<td>0.05</td>
<td>-0.767747961</td>
<td>0.000545020</td>
</tr>
<tr>
<td>40</td>
<td>0.025</td>
<td>-0.767334705</td>
<td>0.000131763</td>
</tr>
<tr>
<td>80</td>
<td>0.0125</td>
<td>-0.767235168</td>
<td>0.000032226</td>
</tr>
<tr>
<td>160</td>
<td>0.00625</td>
<td>-0.767210878</td>
<td>0.000007936</td>
</tr>
<tr>
<td>320</td>
<td>0.003125</td>
<td>-0.767204904</td>
<td>0.000001963</td>
</tr>
</tbody>
</table>
Table 3: The approximate value for the Caputo fractional derivative rule using the backward difference formula: $D_0^\alpha \cos(x)(1)$

<table>
<thead>
<tr>
<th>K</th>
<th>h</th>
<th>$T(f, h, 0.75)$</th>
<th>$T_T(f, h, 0.75)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1</td>
<td>-0.769132238</td>
<td>0.001929296</td>
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<td>0.025</td>
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<td>0.000007846</td>
</tr>
<tr>
<td>320</td>
<td>0.003125</td>
<td>-0.767204893</td>
<td>0.000001951</td>
</tr>
</tbody>
</table>

4 Results and Discussion

Trapezoidal rule is an effective tool for approximation of derivatives and integral of arbitrary order particularly when combined with the finite difference scheme [38]. Engineers and scientist find it useful especially in dealing with problems that are either difficult or cannot be solved analytically, this approach is not only unique but limited in literature and efficient in practice especially when numerical solution is sought, [38], [42], [45].

![Figure 1: This figure shows the convergence to the exact solution as the step size reduces when the trapezoidal rule was modified using the forward, backward and central deference scheme for approximation of $\cos(x)$ at $\alpha = \frac{3}{4}$. Table 1-3 are represented in the graph above.](image)

Our method is for approximation of functions of arbitrary order and for brevity we limit ourselves to $0 < \alpha < 1$. We solve some examples to demonstrate the effectiveness of the algorithm by evaluating the fractional derivative of the function $f(x) = \cos x$ using the modified trapezoidal rule for $\alpha = 0.75$. Table 1 gives the approximate value for the Caputo fractional derivative rule using the central difference, table 2 was evaluated considering the Caputo fractional derivative rule and the forward difference formula while table 3 represent the backward difference scheme with the Caputo fractional derivative rule. Table 1-3 shows the numerical values and errors when compared with the exact solution using the central, forward
and backward difference formula and figure 1 shows the uniform convergence of all three strategies as the step-size decreases. Therefore, we can observe that when $h$ (step size) is reduced by a factor of $1/2$ the successive errors are diminished by approximately $1/4$ this confirms the order is $O(h^2)$ and consistent with the error analysis presented above. This method is effective and consistent especially when compared with other methods and solvers [38–42].

5 Conclusion

Trapezoidal rule has been used in conjunction with the finite difference scheme to derive the computational algorithm for the numerical approximation of Caputo fractional derivative for evaluating functions of arbitrary (real) order. We noticed that the accuracy of the method depends on the step size and the error order of the finite difference scheme and also consistent with current technics and approach.

6 Declarations

6.1 Competing Interests

The author declares no conflict of interest.

6.2 Publisher’s Note

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