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Approximations of fractional integrals and Caputo fractional derivatives

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Abstract

In this paper we propose two algorithms for numerical fractional integration and Caputo fractional differentiation. We present a modification of trapezoidal rule that is used to approximate finite integrals, the new modification extends the application of the rule to approximate integrals of arbitrary order $\alpha > 0$. We then, using the new modification derive an algorithm to approximate fractional derivatives of arbitrary order $\alpha > 0$, where the fractional derivative based on Caputo definition, for a given function by a weighted sum of function and its ordinary derivatives values at specified points. The study is conducted through illustrative examples and error analysis.

Keywords: Fractional integral; Caputo fractional derivative; Modified trapezoidal rule; Caputo fractional derivative rule

1. Introduction

1.1. Trapezoidal rule

Numerical integration is a primary tool used by scientists and engineers to obtain approximate answers for definite integrals that can not be solved analytically. Several methods are used to approximate the definite integral of a given function by a weighted sum of function values at specified points. Trapezoidal rule is based on dividing the area between the curve of $f(x)$ and the x-axis into strips and interpolating the function $f(x)$ by a sequence of straight lines.

Trapezoidal rule. Suppose that the interval $[a,b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of equal width $h = (b-a)/M$ by using the nodes $x_k = a + kh$, for $k = 0, 1, \ldots, M$. The composite trapezoidal rule for the function $f(x)$ over $[a,b]$ is defined as [1,4]

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$$T(f,h) = \frac{h}{2}\sum_{k=1}^{M}(f(x_{k-1}) + f(x_k)) \tag{1.1}$$

$$= \frac{h}{2}(f(a) + f(b)) + h\sum_{k=1}^{M-1} f(x_k). \tag{1.2}$$

This is an approximation to the integral of $f(x)$ over $[a,b]$, and we write

$$\int_a^b f(x)\,\mathrm{d}x \approx T(f,h). \tag{1.3}$$

Trapezoidal rule; *error analysis.* If $f(x) \in \boldsymbol{C}^2\,[a,b]$, then there is a value c with $a < c < b$ so that the error term $E(f,h)$ has the form

$$E(f,h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} = \mathbf{O}(h^2), \tag{1.4}$$

where

$$E(f,h) = \int_a^b f(x)\,\mathrm{d}x - T(f,h). \tag{1.5}$$

1.2. Definitions

Now we will introduce the following definitions and properties of fractional integral and Caputo fractional derivative.

Fractional integral. According to Riemann–Liouville approach to fractional calculus, the fractional integral of order $\alpha > 0$ is defined as [2]

$$J^{\alpha}f(x) = \frac{1}{\Gamma(\alpha)}\int_0^x (x-\tau)^{\alpha-1}f(\tau)\,\mathrm{d}\tau, \quad x > 0. \tag{1.6}$$

Details and properties of the operator J^{α} can be found in [9,11,12], we mention the following:

For $\alpha, \beta > 0$, $x > 0$ and $\gamma > -1$, we have

$$J^{\alpha}J^{\beta} = J^{\alpha+\beta}, \tag{1.7}$$

$$J^{\alpha}x^{\gamma} = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1+\alpha)}x^{\gamma+\alpha}, \tag{1.8}$$

$$J^{\alpha}\mathrm{e}^{ax} = x^{\alpha}\sum_{k=0}^{\infty}\frac{(ax)^k}{\Gamma(\alpha+k+1)}, \tag{1.9}$$

$$J^{\alpha}\cos(ax) = x^{\alpha}\sum_{k=0}^{\infty}\frac{(-1)^k(ax)^{2k}}{\Gamma(\alpha+2k+1)}, \tag{1.10}$$

$$J^{\alpha}\sin(ax) = x^{\alpha}\sum_{k=0}^{\infty}\frac{(-1)^k(ax)^{2k+1}}{\Gamma(\alpha+2k+2)}. \tag{1.11}$$

Caputo fractional derivative. Let m be the smallest integer that exceeds α, then Caputo fractional derivative of order $\alpha > 0$ is defined as [10]

$$D_*^{\alpha}f(x) = J^{(m-\alpha)}[f^{(m)}(x)], \tag{1.12}$$

namely

$$D_*^{\alpha}f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)}\left[\int_0^x \frac{f^{(m)}(\tau)}{(x-\tau)^{\alpha+1-m}}\,\mathrm{d}\tau\right], & m-1 < \alpha < m, \\ \frac{\mathrm{d}^m}{\mathrm{d}x^m}f(x), & \alpha = m. \end{cases} \tag{1.13}$$

1.3. Preliminaries

Formulas for numerical derivatives are important in developing algorithms for solving boundary value problems for ordinary and partial differential equations. Numerical methods for the solution of linear fractional differential equations are well established (see [3,5–8]). Diethelm et al. [8] gives a generalization of Adams–Bashforth–Moulton method to approximate solution of the nonlinear fractional differential equation

$$D_*^{\alpha}y(t) = f(t, y(t)), \quad y(t_0) = y_0, \tag{1.14}$$

which is equivalent to the integral equation

$$y(t) = y(t_0) + \frac{1}{\Gamma(\alpha)}\int_{t_0}^{t}(t-u)^{\alpha-1}f(u, y(u))\,\mathrm{d}u. \tag{1.15}$$

They use the product trapezoidal quadrature formula with respect to the weight function $(t_k - \cdot)^{\alpha-1}$. In other words, they use the approximation

$$\int_{t_0}^{t_k}(t_k-u)^{\alpha-1}f(u)\,\mathrm{d}u \approx \int_{t_0}^{t_k}(t_k-u)^{\alpha-1}\tilde{f}_k(u)\,\mathrm{d}u, \tag{1.16}$$

where $\tilde{f}_k$ is the piecewise linear interpolant for f whose nodes are chosen at the t_j, $j = 0, 1, 2, \ldots, k$. From [8], we take the following result:

Theorem 1. *Suppose that $f \in C^2[0, T]$, $\tilde{f}_k$ is the piecewise linear interpolation for f with nodes chosen at the $t_j = jh$ with $h = T/k$, $j = 0, 1, 2, \ldots, k$, then*

$$\text{(i)} \quad \int_0^{t_k}(t_k-t)^{\alpha-1}\tilde{f}_k(t)\,\mathrm{d}t = \sum_{j=0}^{k}a_{j,k}\cdot f(t_i), \tag{1.17}$$

where

$$a_{j,k} = \frac{h^{\alpha}}{\alpha(\alpha+1)}\begin{cases}(k-1)^{\alpha+1}-(k-1-\alpha)k^{\alpha}, & j=0,\\ (k-j+1)^{\alpha+1}+(k-j-1)^{\alpha+1}-2(k-j)^{\alpha+1}, & 1\leqslant j\leqslant k-1,\\ 1, & j=k,\end{cases} \tag{1.18}$$

$$\text{(ii)} \quad \left|\int_0^{t_k}(t_k-t)^{\alpha-1}f(t)\,\mathrm{d}t - \sum_{j=0}^{k}a_{j,k}\cdot f(t_i)\right| \leqslant C_{\alpha}\|f''\|_{\infty}t_k^{\alpha}h^2, \tag{1.19}$$

for some constant C_{α} depending only on α.

2. Modified trapezoidal rule

In this section, we give a generalization of trapezoidal rule (1.1) to approximate the fractional integral $J^{\alpha}f(x)$ of order $\alpha > 0$.

Theorem 2. *Suppose that the interval $[0, a]$ is subdivided into k subintervals $[x_j, x_{j+1}]$ of equal width $h = a/k$ by using the nodes $x_j = jh$, for $j = 0, 1, \ldots, k$. The modified trapezoidal rule*

$$\begin{aligned}T(f,h,\alpha) = {}&\left((k-1)^{\alpha+1}-(k-\alpha-1)k^{\alpha}\right)\frac{h^{\alpha}f(0)}{\Gamma(\alpha+2)}+\frac{h^{\alpha}f(a)}{\Gamma(\alpha+2)}\\ &+\sum_{j=1}^{k-1}\left((k-j+1)^{\alpha+1}-2(k-j)^{\alpha+1}+(k-j-1)^{\alpha+1}\right)\frac{h^{\alpha}f(x_j)}{\Gamma(\alpha+2)}\end{aligned} \tag{2.1}$$

is an approximation to fractional integral

$$(J^{\alpha}f(x))(a) = T(f,h,\alpha) - E_T(f,h,\alpha), \quad a>0, \ \alpha>0. \tag{2.2}$$

Furthermore, if $f(x) \in \mathbf{C}^2[0,a]$, there is a constant C'_α depending only on α so that the error term $E_T(f,h,\alpha)$ has the form

$$|E_T(f,h,\alpha)| \leqslant C'_\alpha \|f''\|_\infty a^\alpha h^2 = \mathbf{O}(h^2). \tag{2.3}$$

Proof. From definition (1.6), we have

$$(J^\alpha f(x))(a) = \frac{1}{\Gamma(\alpha)} \int_0^a (a-\tau)^{\alpha-1} f(\tau)\,\mathrm{d}\tau. \tag{2.4}$$

If $\tilde{f}_k$ is the piecewise linear interpolant for f whose nodes are chosen at the nodes x_j, $j = 0,1,2,\ldots,k$, then, using (1.17) and (1.19), we obtain

$$\int_0^a (a-\tau)^{\alpha-1} \tilde{f}_k(\tau)\,\mathrm{d}\tau = \frac{h^\alpha}{\alpha(\alpha+1)} \cdot \begin{cases} \left((k-1)^{\alpha+1} - (k-\alpha-1)k^\alpha\right) f(0) + f(a) \\ + \sum_{j=1}^{k-1} \left((k-j+1)^{\alpha+1} - 2(k-j)^{\alpha+1} + (k-j-1)^{\alpha+1}\right) f(x_j) \end{cases} \tag{2.5}$$

and

$$\left| \int_0^a (a-\tau)^{\alpha-1} f(\tau)\,\mathrm{d}\tau - \int_0^a (a-\tau)^{\alpha-1} \tilde{f}_k(\tau)\,\mathrm{d}\tau \right| \leqslant C_\alpha \|f''\|_\infty a^\alpha h^2. \tag{2.6}$$

Therefore, Theorem 2 follows from (2.5) and (2.6) where $C'_\alpha = C_\alpha / \Gamma(\alpha)$. □

It is clear that the behavior of the method is independent of the parameter α and that it behaves in a way that is very similar to the classical trapezoidal rule. In particular, if $\alpha = 1$ the modified trapezoidal rule (2.1) reduces to the trapezoidal rule (1.2).

Example 1. Consider the function $f(x) = \sin x$, in Tables 2.1–2.3 we use the modified trapezoidal rule to approximate the fractional integral $(J^\alpha f(x))(1)$ for different values of α.

Table 2.1
The modified trapezoidal rule for $(J^{0.5} \sin x)(1)$

k	h	$T(f,h,0.5)$	$E_T(f,h,0.5)$
10	0.1	0.6691782509	0.0005060087
20	0.05	0.6695538539	0.0001304057
40	0.025	0.6696509827	0.0000332769
80	0.0125	0.6696758223	0.0000084373
160	0.00625	0.6696821295	0.0000021301

Table 2.2
The modified trapezoidal rule for $(J^1 \sin x)(1)$

k	h	$T(f,h,1)$	$E_T(f,h,1)$
10	0.1	0.4593145489	0.0003831452
20	0.05	0.4596019198	0.0000957743
40	0.025	0.4596737513	0.0000239428
80	0.0125	0.4596917085	0.0000059856
160	0.00625	0.4596961977	0.0000014964

Table 2.3
The modified trapezoidal rule for $(J^{1.5} \sin x)(1)$

k	h	$T(f,h,1.5)$	$E_T(f,h,1.5)$
10	0.1	0.2820860602	0.0002363202
20	0.05	0.2822634794	0.0000589010
40	0.025	0.2823076693	0.0000147111
80	0.0125	0.2823187037	0.0000036767
160	0.00625	0.2823214613	0.0000009191

Note that, using (1.11), the true value of the fractional integral $J^\alpha \sin x$ is

$$J^\alpha \sin x = x^\alpha \sum_{i=0}^{\infty} \frac{(-1)^i x^{2i+1}}{\Gamma(\alpha+2i+2)}, \quad x > 0. \tag{2.7}$$

This value, when $x = 1$, is used to compute the error

$$E_T(f,h,\alpha) = \sum_{i=0}^{\infty} \frac{(-1)^i}{\Gamma(\alpha+2i+2)} - T(f,h,\alpha). \tag{2.8}$$

3. Caputo fractional derivative rule

In this section, we derive an algorithm to approximate Caputo fractional derivatives of arbitrary order $\alpha > 0$ for a given function by a weighted sum of function and its ordinary derivatives values at specified points. Our algorithm is based on the definition (1.3) and modified trapezoidal rule that Caputo fractional derivative for a given function is defined as a finite integral.

Theorem 3. *Suppose that the interval* $[0,a]$ *is subdivided into k subintervals* $[x_j, x_{j+1}]$ *of equal width* $h = a/k$ *by using the nodes* $x_j = jh$, *for* $j = 0,1,\ldots,k$, *then the Caputo fractional derivative rule*

$$C(f,h,\alpha) = \frac{h^{m-\alpha}}{\Gamma(m+2-\alpha)} \left\{ \begin{array}{l} \left((k-1)^{m-\alpha+1} - (k-m+\alpha-1)k^{m-\alpha}\right) f^{(m)}(0) + f^{(m)}(a) \\ \quad + \sum_{j=1}^{k-1} \left((k-j+1)^{m-\alpha+1} - 2(k-j)^{m-\alpha+1} + (k-j-1)^{m-\alpha+1}\right) f^{(m)}(x_j) \end{array} \right. \tag{3.1}$$

is an approximation to the Caputo fractional derivative

$$(D_*^\alpha f(x))(a) = C(f,h,\alpha) - E_C(f,h,\alpha), \quad a > 0, \tag{3.2}$$

for $m-1 < \alpha < m$. *Furthermore, if* $f(x) \in \boldsymbol{C}^{m+2}[0,a]$, *then there is some constant* $C'_{m-\alpha}$ *depending only on* α *so that the error term* $E_C(f,h,\alpha)$ *has the form*

$$|E_C(f,h,\alpha)| \leqslant C'_{m-\alpha} \|f^{(m+2)}\|_\infty a^{m-\alpha} h^2 = \mathbf{O}(h^2). \tag{3.3}$$

Proof. It follows, using the definition (1.13), after replacing α by $m-\alpha$ and $f(\tau)$ by $f^{(m)}(\tau)$ in Theorem 2. □

The reader may notice that we will compute only a finite number of mth ordinary derivatives of the function $f(x)$ at specified points to approximate the Caputo fractional derivative $D_*^\alpha f(x)$ of order α, $m-1 < \alpha < m$.

In case of $0 < \alpha < 1$, then Caputo fractional derivative rule (3.1) reduces to the formula

$$C(f,h,\alpha) = \frac{h^{1-\alpha}}{\Gamma(3-\alpha)} \left\{ \begin{array}{l} \left((k-1)^{2-\alpha} - (k+\alpha-2)k^{1-\alpha}\right) f'(0) + f'(a) \\ \quad + \sum_{j=1}^{k-1} \left((k-j+1)^{2-\alpha} - 2(k-j)^{2-\alpha} + (k-j-1)^{2-\alpha}\right) f'(x_j), \end{array} \right. \tag{3.4}$$

and if $f(x) \in \boldsymbol{C}^3[0,a]$, then the error term $E_C(f,h,\alpha)$ has the form

$$|E_C(f,h,\alpha)| \leqslant C'_{1-\alpha} \|f^{(3)}\|_\infty a^{1-\alpha} h^2, \tag{3.5}$$

for some constant $C'_{1-\alpha}$ depending only on α.

Table 3.1
The Caputo fractional derivative rule for $\left(D_*^{0.5}\sin x\right)(1)$

k	h	$C(f,h,0.5)$	$E_C(f,h,0.5)$
10	0.1	0.8453829878	0.0006737989
20	0.05	0.8458861770	0.0001706097
40	0.025	0.8460137323	0.0000430544
80	0.0125	0.8460459502	0.0000108365
160	0.00625	0.8460540645	0.0000027222

Table 3.2
The Caputo fractional derivative rule for $\left(D_*^{1.5}\sin x\right)(1)$

k	h	$C(f,h,1.5)$	$E_C(f,h,1.5)$
10	0.1	0.6691782509	0.0005060087
20	0.05	0.6695538539	0.0001304057
40	0.025	0.6696509827	0.0000332769
80	0.0125	0.6696758223	0.0000084373
160	0.00625	0.6696821295	0.0000021301

If $1 < \alpha < 2$, then Caputo fractional derivative rule (3.1) reduces to the formula

$$C(f,h,\alpha) = \frac{h^{2-\alpha}}{\Gamma(4-\alpha)}\begin{cases}\left((k-1)^{3-\alpha} - (k+\alpha-3)k^{2-\alpha}\right)f''(0) + f''(a) \\ \quad + \sum\limits_{j=1}^{k-1}\left((k-j+1)^{3-\alpha} - 2(k-j)^{3-\alpha} + (k-j-1)^{3-\alpha}\right)f''(x_j),\end{cases} \tag{3.6}$$

and if $f(x) \in \boldsymbol{C}^4[0,a]$, then the error term $E_C(f,h,\alpha)$ has the form

$$|E_C(f,h,\alpha)| \leqslant C'_{2-\alpha}\|f^{(4)}\|_\infty a^{2-\alpha}h^2, \tag{3.7}$$

for some constant $C'_{2-\alpha}$ depending only on α.

Example 2. Consider the function $f(x) = \sin x$, in Tables 3.1 and 3.2 we use the Caputo fractional derivative rule (3.1) to approximate the fractional derivative $(D_*^\alpha \sin x)(1)$ for some values of α.

Note that, using the definition of Caputo fractional derivative (1.12) and the formulas (1.10) and (1.11), the true value of the Caputo fractional derivative $D_*^\alpha \sin x$ is given by

$$D_*^\alpha \sin x = x^{1-\alpha}\sum_{i=0}^{\infty}\frac{(-1)^i x^{2i}}{\Gamma(2i+2-\alpha)}, \quad \text{for } 0 < \alpha < 1 \tag{3.8}$$

and

$$D_*^\alpha \sin x = x^{2-\alpha}\sum_{i=0}^{\infty}\frac{(-1)^{i+1} x^{2i+1}}{\Gamma(2i+4-\alpha)}, \quad \text{for } 1 < \alpha < 2. \tag{3.9}$$

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