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Author(s)	Sugiura, Hiroshi; Hasegawa, Takemitsu
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Quadrature rule for Abel's equations: uniformly approximating fractional derivatives

Hiroshi Sugiura(Nanzan University)
Takemitsu Hasegawa(University Fukui)

Abstract

An automatic quadrature method is presented for approximating fractional derivative $D^q f(x)$ of a given function $f(x)$, which is defined by an indefinite integral involving $f(x)$. The present method interpolates $f(x)$ in terms of the Chebyshev polynomials in the range $[0,1]$ to approximate the fractional derivative $D^q f(x)$ uniformly for $0 \leq x \leq 1$, namely the error is bounded independently of x. Some numerical examples demonstrate the performance of the present automatic method.

1 Introduction

Fractional calculus (fractional integral and derivative) [6, 14, 17] has been often used recently in modeling many physical and engineering problems, see, say [8, 13, 16] and the references therein, see also [1] for the application in economics. For an interesting history (Leibniz, 30 September 1695) and scientific applications of fractional calculus, see a review due to Cafagna [4].

Let $f(s)$ be a sufficiently well-behaved function in $[0,1]$. The Riemann-Liouville fractional integral $I^{1-q}f(s)$, where $0<q<1$, is defined by

$$I^{1-q}f(s) = \frac{1}{\Gamma(1-q)}\int_0^s f(t)(s-t)^{-q}\,dt, \quad 0<s\leq 1,$$

where $\Gamma(1-q)$ is the gamma function [19]. On the other hand, The fractional derivative $D^q f(s)$ in the Riemann-Liouville version and the Caputo fractional derivative $D_*^q f(s)$ [4, 18] are defined by

$$D^q f(s) = \frac{d}{ds}[I^{1-q}f(s)] = \frac{d}{ds}\Big[\frac{1}{\Gamma(1-q)}\int_0^s f(t)(s-t)^{-q}\,dt\Big], \tag{1}$$

$$D_*^q f(s) = I^{1-q}\Big[\frac{d}{ds}f(s)\Big] = \frac{1}{\Gamma(1-q)}\int_0^s f'(t)(s-t)^{-q}\,dt, \quad 0<s\leq 1, \tag{2}$$

respectively. Riemann-Liouville fractional derivative $D^q f(s)$ differs from $D_*^q f(s)$ as follows,

$$D^q f(s) = f(0)s^{-q}/\Gamma(1-q) + D_*^q f(s). \tag{3}$$

It is well known [2, p.134], [3, p.8], [5] that $D^q f(t)/\Gamma(q)$ gives the solution $y(t)$ of the generalized Abel equation [12, p.174],

$$\int_0^s y(t)(s-t)^{q-1}dt = f(s), \quad 0<q<1, \quad s>0.$$

If $q-1$ is a positive non-integer, then $D^q f(s)$ is defined by

$$D^q f(s) = \frac{d^{m+1}}{ds^{m+1}}[I^{m+1-q}f(s)] = \frac{d^m}{ds^m}[D^{q-m}f(s)],$$

where m is the positive integer such that $m<q<m+1$.

The present method approximates the fractional derivatives $D^q f(s)$ uniformly for $0 < s \le 1$, namely the errors of the approximations are bounded independently of s.

Let $J(s;f)$ be defined by

$$J(s;f) = \Gamma(1-q)\, D_*^q f(s) = \int_0^s f'(t)(s-t)^{-q}\, dt, \tag{4}$$

then from (1), (2) and (3) we see that $D^q f(s)$ can be written by

$$D^q f(s) = \{f(0)s^{-q} + J(s;f)\}/\Gamma(1-q).$$

Approximating $f(t)$, $0 \le t \le 1$, by a sum of the shifted Chebyshev polynomials $T_k(2t-1)$,

$$f(t) \approx p_n(t) = \sum_{k=0}^{n}{}' a_k T_k(2t-1), \quad 0 \le t \le 1, \tag{5}$$

we have an approximation $J(s;p_n)$ to $J(s;f)$ as follows,

$$J(s;f) \approx J(s;p_n) = \int_0^s p_n'(t)(s-t)^{-q}\, dt. \tag{6}$$

In (5) the prime denotes the summation whose first term is halved. The Chebyshev coefficients a_k in (5) can be determined so that $p_n(t)$ may interpolate $f(t)$ at abscissae $t_j = \{1 + \cos(\pi j/n)\}/2$, $j = 0, \ldots, n$, [20] as follows

$$a_k = \frac{2\delta_k}{n} \sum_{j=0}^{n}{}'' f(t_j) \cos\frac{\pi j k}{n},$$

where $\delta_k = 1$, $(k = 0 \ldots, n-1)$, $\delta_n = 0.5$ and the double prime denotes the summation whose first and last terms are halved, and can be efficiently evaluated by using the FFT [11]. If $f(t)$ is a smooth function, then the sum of the Chebyshev polynomials (5) converges to $f(t)$ quickly as $n \to \infty$ [20].

To evaluate $J(s;p_n)$ given by (6) we use a polynomial $F_{n-1}(t)$ of degree $n-1$ to write

$$\int_x^s \{p_n'(s) - p_n'(t)\}(s-t)^{-q} dt = \{F_{n-1}(s) - F_{n-1}(x)\}(s-x)^{1-q}. \tag{7}$$

From (7) we have

$$J(s;p_n) = \int_0^s p_n'(t)(s-t)^{-q} dt = \left[\frac{p_n'(s)}{1-q} - F_{n-1}(s) + F_{n-1}(0)\right] s^{1-q}, \tag{8}$$

and the approximation $\widetilde{D}_n^q f(s)$ to $D^q f(s)$ as follows

$$\widetilde{D}_n^q f(s) = \{f(0)s^{-q} + J(s;p_n)\}/\Gamma(1-q).$$

Functions $p_n'(t)$ and $F_{n-1}(t)$ of degree $n-1$ are also expanded in terms of the shifted Chebyshev polynomials, see section 2.

This paper is organized as follows. In section 2 we express $F_{n-1}(t)$ in (7) by a sum of the Chebyshev polynomials and show the recurrence relation satisfied by the Chebyshev coefficients. In section 3 we estimate the error of the approximation to the fractional derivative, in particular to $J(s;f)$. In section 4 numerical examples are shown to demonstrate the performance of the present automatic quadrature method.

2 Evaluation of $F_{n-1}(t)$

Differentiating both sides of (7) with respect to x yields

$$\begin{aligned}&\{p_n'(s) - p_n'(x)\}(s-x)^{-q}\\&= F_{n-1}'(x)(s-x)^{1-q} + \{F_{n-1}(s) - F_{n-1}(x)\}(1-q)(s-x)^{-q},\end{aligned}$$

namely we have

$$p_n'(s) - p_n'(x) = F_{n-1}'(x)(s-x) + \{F_{n-1}(s) - F_{n-1}(x)\}(1-q). \tag{9}$$

To evaluate $F_{n-1}(s)$ in (8) we expand $F_{n-1}'(x)$ in terms of the shifted Chebyshev polynomials

$$F_{n-1}'(x) = \sum_{k=0}^{n-2}{}' b_k T_k(2x-1), \quad 0 \le x \le 1, \tag{10}$$

where we have omitted the dependency of b_k on s. Integrating both sides of (10) gives

$$F_{n-1}(x) - F_{n-1}(s) = \sum_{k=1}^{n-1} \frac{b_{k-1} - b_{k+1}}{4k}\{T_k(2x-1) - T_k(2s-1)\}, \tag{11}$$

where we define $b_{n-1} = b_n = 0$. On the other hand, by using the relation $T_{k+1}(u) + T_{k-1}(u) = 2uT_k(u)$, $-1 \le u \le 1$, we have

$$\begin{aligned}(x-s)F_{n-1}'(x) &= F_{n-1}'(x)\{(2x-1) - (2s-1)\}/2\\&= \frac{1}{4}\sum_{k=0}^{n-1}{}' \{b_{k+1} - 2(2s-1)b_k + b_{k-1}\}T_k(2x-1),\end{aligned} \tag{12}$$

where we set $b_{-1} = b_1$. Further by inserting $F_{n-1}(x) - F_{n-1}(s)$ and $(x-s)F_{n-1}'(x)$ given by (11) and (12), respectively and $p_n'(x)$ written by

$$p_n'(x) = \sum_{k=0}^{n-1}{}' c_k T_k(2x-1), \tag{13}$$

into (9) we have

$$\left\{1 - \frac{1-q}{k}\right\}b_{k+1} - 2(2s-1)\,b_k + \left\{1 + \frac{1-q}{k}\right\}b_{k-1} = 4\,c_k, \quad 1 \le k. \tag{14}$$

We can stably compute the recurrence relation (14) in the backward direction with starting values $b_n = b_{n-1} = 0$ to obtain b_k, $k = n-2, \ldots, 0$. The Chebyshev coefficients c_k of $p_n'(x)$ given by (13) can be evaluated by the relation [15]

$$c_{k-1} = c_{k+1} + 4\,k\,a_k, \quad k = n, n-1, \ldots, 1,$$

with starting values $c_n = c_{n+1} = 0$, where a_k are the Chebyshev coefficients of $p_n(x)$ in (5).

3 Error estimate

We estimate the error of the approximation to the fractional derivative $D^q f(s)$, particularly the error of $J(s; p_n)$. We shall use the notation that for $n >> 1$, $a(n) \sim b(n)$ and $a(n) \lesssim b(n)$ mean that $\lim_{n\to\infty} a(n)/b(n) = 1$ and $\lim_{n\to\infty} a(n)/b(n) \le 1$, respectively. Let $\omega_{n+1}(t)$ be defined by

$$\omega_{n+1}(t) = T_{n+1}(2t-1) - T_{n-1}(2t-1), \tag{15}$$

then $p_n(t)$ agrees with $f(t)$ at the zeros of $\omega_{n+1}(t)$, namely $\{1+\cos(\pi j/n)\}/2$, $0 \le j \le n$. Let $\mathcal{E}_\rho$ denote the ellipse in the complex plane $z = x + iy$,

$$\mathcal{E}_\rho : \quad z = (w + w^{-1} + 2)/4, \quad w = \rho e^{i\theta}, \quad 0 \le \theta \le 2\pi, \tag{16}$$

with foci at $z = 0, 1$ and the sum of its major and minor axes equal to $\rho(> 1)$. We have the following theorem.

Theorem 3.1 *Suppose that $f(z)$ is single-valued and analytic inside and on $\mathcal{E}_\rho$ defined by (16) and let $K = \max_{z\in\mathcal{E}_\rho} |f(z)|$. Then the approximation $J(s;p_n)$ given by (6) uniformly converges to $J(s;f)$ given by (4) as $n \to \infty$ as follows,*

$$|J(s;f) - J(s;p_n)| \le \frac{16K\{n(\rho-1)^2+\rho\}\rho}{(1-q)\,(\rho-1)^4\,(\rho^n-\rho^{-n})} = O(n\rho^{-n}), \ \rho > 1. \tag{17}$$

Since our goal is to construct an automatic quadrature method, we wish to estimate the error of the approximation $J(s;p_n)$ (8) in terms of the available coefficients a_k of $p_n(t)$. Suppose that $f(z)$ is a meromorphic function which has only simple pole at the point $z = \alpha \equiv (\beta + \beta^{-1} + 2)/4$ in an ellipse $\mathcal{E}_\sigma$, $1 < \rho < \sigma$, where $1 < \rho < |\beta| < \sigma$. We have an estimated error $E_n(f)$ for the approximation $J(s;p_n)$

$$|J(s;f) - J(s;p_n)| \le \frac{8nL_n + 2L_n'}{1-q} \sim \frac{8nL_n}{1-q} \lesssim \frac{8rn|a_n|}{(1-q)\,(r-1)^2} \equiv E_n(f), \tag{18}$$

where $r = |\beta|$.
Remark. The constant r may be estimated from the asymptotic behavior of $\{a_k\}$ [10].

Incidentally, an automatic quadrature of nonadaptive type is constructed from the sequence of the approximations $\{J(s;p_n)\}$ converging the integral $J(s;f)$, until a stopping criterion is satisfied. It is an usual and simple way to double the degree n of $p_n(t)$ (5) for generating the sequence $\{J(s;p_n)\}$ (8), see [9]. In order to make an automatic quadrature efficient, however, it is advantageous to have more chance of checking the stopping criterion than doubling n. To this end, as is shown in [11] we may generate the sequence of $\{p_n\}$, increasing the degree n more slowly as follows:

$$n = 6, 8, 10, \ldots, 3\times 2^i, 4\times 2^i, 5\times 2^i, \ldots, \quad (i = 1, 2, 3, \ldots)$$

and by using the FFT.
Stopping rule. We compute the sequence of $\{p_n(t)\}$ until $E_n(f)/\Gamma(1-q)$, where $E_n(f)$ is given by (18), is less than or equal to the required tolerance ε for $D^q f(t)$.

4 Numerical examples

Table 1: Approximations of $D^{1/2}(s+0.1)^{-0.5}$ with the required tolerance $\varepsilon = 10^{-6}$ for $0 \le s \le 1$. The number $n+1$ of function evaluations required to satisfy ε is 41.

s	approximation	error
0.09	3.1300423140*508*	0.35E−10
0.29	0.8494962341*923*	0.63E−10
0.49	0.43199131159*67*	0.48E−11
0.69	0.2718775997*025*	0.41E−10
0.89	0.19102704860*19*	0.84E−11

Examples in this section were computed in double precision: the machine precision is $2.22\ldots\times 10^{-16}$.

Table 2: Approximations for $D^q(s+a)^{q-1}$, $0 \le s \le 1$. The numbers $n+1$ of function evaluations required to satisfy the tolerances $\varepsilon = 10^{-5}$ and 10^{-9} are listed in the third and fifth columns, respectively. The actual maximum errors E_n in magnitude of approximations for $0 \le s \le 1$ are listed in the fourth and sixth columns.

		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-9}$	
q	a	$n+1$	E_n	$n+1$	E_n
	0.01	129	6.8E−10	161	3.4E−12
0.1	0.1	33	1.9E−8	49	2.6E−12
	1.0	13	8.8E−10	17	2.9E−13
	0.01	97	6.4E−7	161	2.3E−12
0.5	0.1	33	1.3E−8	49	1.7E−12
	1.0	13	7.2E−10	17	2.7E−13
	0.01	81	2.7E−6	129	1.0E−10
0.9	0.1	33	3.6E−9	49	3.6E−13
	1.0	13	3.3E−10	17	9.9E−14

Table 3: Approximations for $D^q e^{a(s-1)}$ with the required tolerances $\varepsilon = 10^{-5}$ and 10^{-9}

		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-9}$	
q	a	$n+1$	E_n	$n+1$	E_n
	1	9	3.4E−11	13	7.8E−16
0.1	6	17	8.9E−13	21	2.4E−15
	11	17	3.0E−9	25	5.9E−15
	1	9	1.0E−10	13	1.3E−15
0.5	6	17	3.6E−12	21	7.5E−15
	11	21	1.1E−11	25	1.2E−14
	1	11	4.9E−13	13	1.1E−14
0.9	6	17	2.5E−11	21	7.2E−14
	11	21	5.4E−11	25	9.0E−14

We compute $D^q f(s)$ for four types of $f(s)$, where (A) $f(s) = (s+a)^{q-1}$, (B) $f(s) = e^{a(s-1)}$, (C) $f(s) = \sin as$, and (D) $f(s) = s^{a/2} J_a(2\sqrt{s})$ and (E) $D^{1/2} f(s)$ where $f(s) = 1/(s^2+a^2)$. The exact values of the fractional derivatives of these functions are given, respectively, by

$$\text{(A)} \qquad D^q(s+a)^{q-1} = \frac{1}{\Gamma(1-q)} \left(\frac{a}{s}\right)^q \frac{1}{s+a},$$

$$\text{(B)} \qquad D^q e^{a(s-1)} = e^{-a} s^{-q} \sum_{k=0}^{\infty} \frac{(as)^k}{\Gamma(k-q+1)},$$

$$\text{(C)} \qquad D^q \sin as = a\, s^{1-q} \sum_{k=0}^{\infty} \frac{(-1)^k (as)^{2k}}{\Gamma(2k+2-q)},$$

$$\text{(D)} \qquad D^q s^{a/2} J_a(2\sqrt{s}) = s^{(a-q)/2} J_{a-q}(2\sqrt{s}),$$

$$\text{(E)} \qquad D^{1/2}\left\{\frac{1}{s^2+a^2}\right\} = \frac{1}{\sqrt{\pi s}\,(s^2+a^2)} - \frac{1}{\sqrt{\pi}\, a} \Im\left\{\frac{\sin^{-1}\sqrt{s/(ia)}}{(ia-s)^{3/2}}\right\}.$$

Table 1 shows the approximations $\widetilde{D}_n^{1/2}(s+0.1)^{-0.5}$ and actual errors $|D^{1/2}(s+0.1)^{-0.5} - \widetilde{D}_n^{1/2}(s+0.1)^{-0.5}|$ with the required tolerance $\varepsilon = 10^{-6}$ for $s = 0.09 + i/5$, $i = 0, 1, \ldots, 4$. The number $n+1$ of

Table 4: Approximations for $D^q \sin as$ with the required tolerances $\varepsilon = 10^{-5}$ and 10^{-9}

		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-9}$	
q	a	$n+1$	E_n	$n+1$	E_n
	1	9	4.8E−11	13	4.4E−16
0.1	8	17	1.1E−9	25	5.8E−14
	15	25	5.8E−11	33	3.5E−11
	1	9	1.5E−10	13	8.9E−16
0.5	8	17	4.6E−9	25	1.1E−13
	15	25	2.8E−10	33	1.2E−10
	1	11	7.0E−13	13	4.4E−15
0.9	8	21	6.2E−12	25	2.5E−13
	15	25	1.4E−9	33	4.4E−10

Table 5: Approximations for $D^q \sqrt{s}^a J_a(2\sqrt{s})$ with the required tolerances $\varepsilon = 10^{-5}$ and 10^{-9}

		$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-9}$	
q	a	$n+1$	E_n	$n+1$	E_n
	1.5	97	1.6E−7	1025	2.5E−11
0.1	2.0	9	1.0E−14	11	2.2E−16
	2.5	25	5.2E−8	129	7.2E−12
	1.5	129	1.1E−6	1025	*1.1*E−9*
0.5	2.0	9	3.1E−14	11	3.3E−16
	2.5	33	8.6E−8	129	1.1E−10
	1.5	161	*1.6*E−5*	1537	*2.1*E−8*
0.9	2.0	9	1.5E−13	11	1.9E−15
	2.5	33	1.2E−6	161	*1.2*E−9*

Asterisk means the failure to satisfy the tolerances ε.

function evaluations required is 41. Table 2 also shows the result for the problem (A) with varied values of q and a, namely the numbers $n+1$ required to satisfy the tolerances $\varepsilon = 10^{-5}$ and 10^{-9} and the actual maximum errors E_n defined by

$$E_n = \max_{1 \le j \le m} |D^q f(s_j) - \widetilde{D}_n^q f(s_j)|, \quad s_j = j/m, \quad j = 1, 2, \ldots, m,$$

where we choose large m, say, $m = 1000$. Tables 3∼6 show the results for the problems (B)∼(E), respectively.

From Tables 2∼6 we see that the present automatic method could approximate successfully the fractional derivatives (A)∼(D) with varied values of q and a and (E) with varied values of a for $q = 1/2$ except for (D) with $a = 1.5$ and $q = 0.5, 0.9$ for $\varepsilon = 10^{-9}$, with $a = 1.5$ and $q = 0.9$ for $\varepsilon = 10^{-5}$ and with $a = 2.5$ and $q = 0.9$ for $\varepsilon = 10^{-9}$. The present method is not suitable for the functions with a singularity in $[0, 1]$ or singularities of higher-order derivatives. Indeed, as seen from Table 5, the present method sometimes fails to approximate the fractional derivatives of Bessel functions $s^{a/2} J_a(2\sqrt{s})$ of $a = 1.5$ and 2.5 since Bessel functions $J_a(s)$ of fractional orders a have discontinuous derivatives of higher order at $s = 0$.

Table 6: Approximations for $D^{1/2}\{1/(s^2+a^2)\}$ with the required tolerances $\varepsilon = 10^{-5}$ and 10^{-9}

	$\varepsilon = 10^{-5}$		$\varepsilon = 10^{-9}$	
a	$n+1$	E_n	$n+1$	E_n
1	17	1.0E−10	21	1.8E−13
1/4	33	1.2E−8	49	1.3E−13
1/16	81	5.2E−9	97	1.8E−11

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