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Takemitsu Hasegawa [a,*] Hiroshi Sugiura [b]

[a] *Department of Information Science*
University of Fukui, Fukui, 910-8507, Japan

[b] *Department of Information Systems and Mathematical Sciences*
Nanzan University, Seto, Aichi, 489-0863, Japan

Abstract

Fractional derivative $D^q f(x)$ $(0 < q < 1,\ 0 \le x \le 1)$ of a function $f(x)$ is defined in terms of an indefinite integral involving $f(x)$. For functions of algebraic singularity $f(x) = x^\alpha g(x)$ $(\alpha > -1)$ with $g(x)$ being a well-behaved function, we propose a quadrature method for uniformly approximating $D^q\{x^\alpha g(x)\}$. Present method consists of interpolating $g(x)$ at abscissae in $[0, 1]$ by a finite sum of Chebyshev polynomials. It is shown that the use of the lower endpoint $x = 0$ as an abscissa is essential for the uniform approximation, namely to bound the approximation errors independently of $x \in [0, 1]$. Numerical examples demonstrate the performance of the present method.

Key words: fractional derivative, algebraic singularity, uniform approximation, quadrature rule, Chebyshev interpolation, automatic quadrature, error analysis, five-term recurrence relation

1 Introduction

The fractional derivative and integral equations including fractional derivatives have a long history and have often appeared in science, engineering and finance, see, say Gorenflo and Mainardi [9], while approximation methods have been developed recently. Let $f(s)$ be a given function for $s \in [0, 1]$. The

* Corresponding author.
Email addresses: hasegawa@fuis.fuis.fukui-u.ac.jp (Takemitsu Hasegawa), sugiurah@ms.nanzan-u.ac.jp (Hiroshi Sugiura).

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fractional derivative in the Riemann-Liouville version $D^q f(s)$ and the Caputo version $D^q_* f(s)$ $(0 < q < 1)$ are defined by, respectively, with a relation between them [16]

$$D^q f(s) = \frac{1}{\Gamma(1-q)} \cdot \frac{d}{ds} \int_0^s f(t)(s-t)^{-q}\, dt, \quad 0 \le s \le 1, \quad 0 < q < 1, \tag{1}$$

$$D^q_* f(s) = \frac{1}{\Gamma(1-q)} \int_0^s f'(t)(s-t)^{-q}\, dt = D^q f(s) - \frac{s^{-q} f(0)}{\Gamma(1-q)}. \tag{2}$$

There is comprehensive literature on the numerical methods for solving equations involving fractional derivatives and integrals [2–6,12,14,15]. In contrast, it appears that little literature exists on automatic quadratures for the fractional derivative except for our recent scheme [16] for $D^q f(s)$ $(0 < q < 1)$ of a well-behaved function $f(s)$. In practical applications, however, it is required to approximate the fractional derivatives of badly-behaved functions of various types or functions with singularities [1,8] such that $f(s) = s^\alpha g(s)$, $\alpha > -1$, where $g(s)$ is assumed to be a well-behaved function, see Piessens [15].

The purpose of this paper is to extend our previous paper [16] to approximate $D^q\{s^\alpha g(s)\}$ given by, with the required tolerance ε

$$D^q\{s^\alpha g(s)\} = \frac{1}{\Gamma(1-q)} \cdot \frac{d}{ds} \int_0^s g(t)\, t^\alpha (s-t)^{-q} dt, \tag{3}$$
$$0 < q < 1, \quad \alpha \ge q-1, \quad 0 \le s \le 1.$$

We approximate $g(t)$ in (3) by a sum of the shifted Chebyshev polynomials $T_k(2t-1)$,

$$g(t) \approx p_n(t) = {\sum_{k=0}^{n}}{}' \, a_k\, T_k(2t-1), \quad 0 \le t \le 1. \tag{4}$$

where the prime denotes the summation whose first term is halved. Then we have an approximation $D^q_n\{s^\alpha g(s)\}$ to $D^q\{s^\alpha g(s)\}$ as follows,

$$D^q_n\{s^\alpha g(s)\} := D^q\{s^\alpha p_n(s)\} = \frac{1}{\Gamma(1-q)} \cdot \frac{d}{ds} \int_0^s p_n(t)\, t^\alpha (s-t)^{-q}\, dt. \tag{5}$$

The coefficients a_k are determined so that $p_n(t)$ interpolates $g(t)$ at the points $t_j = \{1+\cos(\pi j/n)\}/2$ $(0 \le j \le n)$, namely $a_k = (2\delta_k/n) \sum_{j=0}^{n}{}'' g(t_j) \cos \pi jk/n$, where $\delta_k = 1$ $(0 \le k \le n-1)$, $\delta_n = 0.5$ and the double prime denotes the summation whose first and last terms are halved, and can be efficiently evaluated by using the FFT [7,11,18]. Note that $p_n(0) = g(0)$ and $p_n(1) = g(1)$.

Let $h_{n-1}(t)$ be a polynomial of degree $n-1$ defined by

$$p_n(t) = t\,h_{n-1}(t) + p_n(0) = t\,h_{n-1}(t) + g(0). \tag{6}$$

Then since $p_n'(t) = h_{n-1}(t) + th_{n-1}'(t)$ and $t^{\alpha+1}h_{n-1}(t) = 0$ when $t = 0$, substituting $p_n(t)$ above in (5) we have

$$\begin{aligned} D^q\{s^\alpha p_n(s)\} - g(0)D^q s^\alpha &= D^q\{s^{\alpha+1}h_{n-1}(s)\} = D_*^q\{s^{\alpha+1}h_{n-1}(s)\} \\ &= \frac{1}{\Gamma(1-q)}\int_0^s \{(\alpha+1)h_{n-1}(t) + th_{n-1}'(t)\}t^\alpha(s-t)^{-q}dt \\ &= \frac{1}{\Gamma(1-q)}\int_0^s \{\alpha h_{n-1}(t) + p_n'(t)\}t^\alpha(s-t)^{-q}dt, \end{aligned} \tag{7}$$

where $D_*^q\{s^{\alpha+1}h_{n-1}(s)\}$ denotes the Caputo fractional derivative (2). To evaluate the integral in the rightmost hand of (7) we need the following lemma.

Lemma 1.1 *For the polynomial $h_{n-1}(t)$ (6) there exist polynomials $F_{n-2}(t)$ of degree $n-2$ and $G_{n-1}(s)$ of degree $n-1$ such that*

$$\int_x^s \frac{\{\alpha h_{n-1}(t) + p_n'(t)\}\,t^\alpha}{(s-t)^q}dt = \frac{x^{\alpha+1}F_{n-2}(x)}{(s-x)^{q-1}} + G_{n-1}(s)\int_x^s \frac{t^\alpha}{(s-t)^q}dt. \tag{8}$$

Proof Let $\mu_k = \int_x^s t^{k+\alpha}(s-t)^{-q}\,dt$. Then, since $d[t^{k+\alpha}(s-t)^{1-q}]/dt = \{(k+\alpha)\,s - (k+\alpha-q+1)\,t\}t^{k+\alpha-1}(s-t)^{-q}$, we have

$$\mu_k = [\{x^{\alpha+1}(s-x)^{1-q}\}\,x^{k-1} + (k+\alpha)\,s\,\mu_{k-1}]\big/(k+\alpha-q+1). \tag{9}$$

The repeated use of the recurrence relation (9) yields

$$\mu_k = x^{\alpha+1}(s-x)^{1-q}\psi_{k-1}(x) + A_k s^k \mu_0, \tag{10}$$

where $\psi_k(x)$ is a polynomial of degree k and A_k is a constant independent of x and s. We define $\psi_{-1}(x) = 0$. Noting that the left hand side of (8) can be written in the form $\sum_{k=0}^{n-1}\beta_k\mu_k$, where β_k are constants, and using (10), we can establish (8). $\square$

The function $F_{n-2}(t)$ in (8) is also expanded in terms of the shifted Chebyshev polynomials, see (14) and (15) in section 2. From (8) we have

$$\int_0^s \{\alpha h_{n-1}(t) + p_n'(t)\}\, t^\alpha (s-t)^{-q} dt = G_{n-1}(s)\, s^{\alpha-q+1} B(\alpha+1, 1-q), \quad (11)$$

since $\int_0^s t^\alpha (s-t)^{-q} = s^{\alpha+1-q} B(\alpha+1, 1-q)$ where $B(\alpha+1, 1-q)$ is the beta integral. Since $B(\alpha+1, 1-q) = \Gamma(\alpha+1)\Gamma(1-q)/\Gamma(\alpha-q+2)$ and $D^q s^\alpha = s^{\alpha-q}\,\Gamma(\alpha+1)/\Gamma(\alpha+1-q)$, from (5), (7) and (11) we have

$$D_n^q\{s^\alpha g(s)\} = \{G_{n-1}(s)\, s + (\alpha-q+1)\, g(0)\} \frac{s^{\alpha-q}\,\Gamma(\alpha+1)}{\Gamma(\alpha-q+2)}. \quad (12)$$

This paper is organized as follows. In section 2 we express the derivative $F_{n-2}'(t)$ of $F_{n-2}(x)$ in (8) by a sum of the Chebyshev polynomials whose coefficients satisfy a five-term inhomogeneous recurrence relation. In section 3 the stability analysis of the recurrence relation is given. We show that a non-dominant solution of the recurrence relation gives the required Chebyshev coefficients of $F_{n-2}'(t)$ as well as the value of $G_{n-1}(s)$ and is obtained in a numerically stable way by the computation of the recurrence relation in the backward direction. In section 4 we estimate the error of the approximation $D_n^q\{s^\alpha g(s)\}$ (12) and show that the use of the lower endpoint $t = 0$ as an abscissa in the integration rule is essential to uniformly bound the errors of $D_n^q\{s^\alpha g(s)\}$ for $0 \le s \le 1$. Section 5 shows numerical examples to demonstrate the performance of the present method.

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

From the differentiated result of both sides of (8) with respect to x we have

$$\begin{aligned} \alpha h_{n-1}(x) + p_n'(x) = {} & \{(\alpha+2-q)x - (\alpha+1)s\} F_{n-2}(x) \\ & + x(x-s) F_{n-2}'(x) + G_{n-1}(s). \end{aligned} \quad (13)$$

To evaluate $F_{n-2}(x)$ and $G_{n-1}(s)$ in (13) we expand $F_{n-2}'(x)$ in terms of the shifted Chebyshev polynomials

$$F_{n-2}'(x) = \sum_{k=0}^{n-3}{}' \, b_k\, T_k(2x-1), \quad 0 \le x \le 1, \quad (14)$$

where we have omitted the dependency of b_k on s. In the sequel we define $b_k = 0$ $(k \geq n-2)$ for convenience. Integrating both sides of (14) gives

$$F_{n-2}(x) = \sum_{k=1}^{n-2} \frac{b_{k-1} - b_{k+1}}{4k} T_k(2x-1) + \gamma, \tag{15}$$

with some constant γ independent of x and s. By using the relation $T_{|k+1|}(u) + T_{|k-1|}(u) = 2uT_{|k|}(u)$, $u = 2x-1$, in (14) and (15) we have

$$\begin{aligned} 16x(x-s)F'_{n-2}(x) &= \sum_{k=0}^{n-1}{}' \{b_{k+2} + 4(1-s)(b_{k+1} + b_{|k-1|}) \\ &\quad +2(3-4s)b_k + b_{|k-2|}\} T_k(2x-1), \qquad (16) \\ 16xF_{n-2}(x) &= \sum_{k=2}^{n-1} \Big\{\frac{b_{k-2}}{k-1} + 2\frac{b_{k-1} - b_{k+1}}{k} - \frac{2b_k}{k^2-1} - \frac{b_{k+2}}{k+1}\Big\} T_k(2x-1) \\ &\quad + \Big(8\gamma + \frac{b_1 - b_3}{2} + 2b_0 - 2b_2\Big) T_1(2x-1) + 8\gamma + b_0 - b_2. \qquad (17) \end{aligned}$$

By inserting in (13), $F_{n-2}(x)$ (15), $x(x-s)F'_{n-2}(x)$ (16) and $xF_{n-2}(x)$ (17), and $p'_n(x)$ and $h_{n-1}(x)$ written by

$$p'_n(x) = \sum_{k=0}^{n-1}{}' c_k T_k(2x-1), \quad h_{n-1}(x) = \sum_{k=0}^{n-1}{}' d_k T_k(2x-1), \tag{18}$$

we have the followings. Let $\beta = \alpha + 2 - q$ and $L(b_k)$ $(2 \leq k \leq n-1)$ be defined by

$$\begin{aligned} L(b_k) &= \Big(1 - \frac{\beta}{k+1}\Big) b_{k+2} + 2\Big\{2 - 2s + \frac{2(\alpha+1)s - \beta}{k}\Big\} b_{k+1} \\ &\quad +2\Big(3 - 4s - \frac{\beta}{k^2-1}\Big) b_k + 2\Big\{2 - 2s - \frac{2(\alpha+1)s - \beta}{k}\Big\} b_{k-1} \qquad (19) \\ &\quad +\Big(1 + \frac{\beta}{k-1}\Big) b_{k-2}, \end{aligned}$$

then we have

$$\begin{aligned} & L(b_k) = 16(\alpha d_k + c_k), \quad 2 \leq k \leq n-1, \qquad (20) \\ & (1-\beta/2)b_3 + 2(2 - \beta + 2\alpha s)b_2 + (7 - 8s + \beta/2)b_1 \\ & \quad +2\{2 + \beta - 2(\alpha+2)s\}b_0 + 8\beta\gamma = 16(\alpha d_1 + c_1), \qquad (21) \\ & (1-\beta)b_2 + 4(1-s)b_1 + (3 - 4s + \beta)b_0 + 8\{\beta - 2(\alpha+1)s\}\gamma, \\ & \quad +16G_{n-1}(s) = 8(\alpha d_0 + c_0). \qquad (22) \end{aligned}$$

The coefficients c_k of $p_n'(x)$ (18) can be evaluated by the relation [13, p.34]

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

with starting values $c_n = c_{n+1} = 0$, where a_k are the Chebyshev coefficients of $p_n(x)$ in (4). The coefficients d_k of $h_{n-1}(t)$ are computed by the relation

$$d_{k+1} + 2d_k + d_{k-1} = 4a_k, \qquad k = n, n-1, \ldots, 1, \tag{23}$$

with starting values $d_{n+1} = d_n = 0$. The relation (23) is derived by using (4) and (18) in (6). Computing the recurrence relation (20), (21) and (22) in the backward direction with starting values $b_{n-2} = b_{n-1} = b_n = b_{n+1} = 0$ in a stable way as shown below gives the required value of $G_{n-1}(s)$ (12).

3 Stability analysis of the solution by the recurrence relation

The required solution b_k of the fourth-order inhomogeneous difference equation (20) is a particular solution w_k which is dominated by a fundamental set [19, p.266] $\{y_k^{(i)}\}_{i=1}^4$, of the homogeneous difference equation $L(y_k) = 0$, where $L(b_k)$ is defined by (19). In fact, the characteristic equation [19, p.270] for $L(b_k) = 0$ is given by

$$\begin{aligned} 0 &= t^4 + 4(1-s)(t^3+t) + 2(3-4s)t^2 + 1 \\ &= (t+1)^2\{t^2 + 2(1-2s)t + 1\} = \prod_{j=1}^{4}(t - t_j), \end{aligned} \tag{24}$$

where $t_1 = t_2 = -1$, $t_3 = e^{i\theta}$ and $t_4 = e^{-i\theta}$ and we defined $\theta = \arctan\{2\sqrt{s(1-s)}\,/(2s-1)\}$.

Lemma 3.1 *Let t_j be zeros of (24) and $L(b_k)$ be defined by (19). Then each $y_k^{(i)}$ of the fundamental set for $L(b_k) = 0$ has the property*

$$\lim_{k\to\infty} y_{k+1}^{(i)}/y_k^{(i)} = t_i, \quad 1 \le i \le 4.$$

Proof. See Theorem B.2 in Wimp [19, p.270]. □

Since the required solution w_k of (20) goes to 0 when $k \to \infty$, it follows from Lemma 3.1 that

$$\lim_{k\to\infty} w_k/y_k^{(i)} = 0, \quad 1 \le i \le 4,$$

which implies that the backward recursion of (20), (21) and (22) is numerically stable to compute w_k.

4 Error estimate

We estimate the error of the approximation $D_n^q\{s^\alpha g(s)\}$ (12). 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 $\lim_{n\to\infty} a(n)/b(n) \leq 1$, respectively.

Let $\omega_{n+1}(t)$ be defined by

$$\omega_{n+1}(t) = T_{n+1}(2t-1) - T_{n-1}(2t-1) = 8t\,(t-1)\,U_{n-1}(2t-1), \qquad (25)$$

where $U_n(x)$ is the Chebyshev polynomial of the second kind, then $p_n(t)$ agrees with $g(t)$ at the zeros of $\omega_{n+1}(t)$, namely $\{1+\cos(\pi j/n)\}/2$, $0 \leq j \leq n$. Let $\mathcal{E}_\rho$ denote the ellipse in the complex plane $z = x + iy$,

$$\mathcal{E}_\rho: \quad z = (w + w^{-1} + 2)/4, \quad w = \rho\, e^{i\theta}, \quad 0 \leq \theta < 2\pi, \qquad (26)$$

with foci at $z = 0, 1$ and the sum of its major and minor axes equal to $\rho(> 1)$. Assume that $g(z)$ is single-valued and analytic inside and on $\mathcal{E}_\rho$. Then the error of $p_n(t)$ can be expressed in terms of contour integral as follows [16]

$$g(t) - p_n(t) = \omega_{n+1}(t) V_n(t), \qquad V_n(t) \equiv \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{g(z)\, dz}{(z-t)\,\omega_{n+1}(z)}. \qquad (27)$$

The following lemma shows that the abscissa at endpoint $t = 0$ in (25) plays an important role in the uniform bound of the errors of the approximations $D_n^q\{s^\alpha g(s)\}$.

Lemma 4.1 *Let $L_n = \max_{0\leq t\leq 1} |V_n(t)|$ and $L_n' = \max_{0\leq t\leq 1} |V_n'(t)|$. Then the error of the approximation $D_n^q\{s^\alpha g(s)\}$ to $D^q\{s^\alpha g(s)\}$ for $0 < q < 1$ is bounded independently of s for $0 \leq s \leq 1$ and for $\alpha + 1 - q \geq 0$, as follows,*

$$|D^q\{s^\alpha g(s)\} - D_n^q\{s^\alpha g(s)\}| \leq 2\{4n(\alpha+1)L_n + L_n'\} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+2-q)}. \qquad (28)$$

Proof Recalling that $D_n^q\{s^\alpha g(s)\} = D^q\{s^\alpha p_n(s)\}$ and from (27) we have

$$D^q\{s^\alpha g(s)\} - D_n^q\{s^\alpha g(s)\} = D^q[s^\alpha\{g(s) - p_n(s)\}]$$

$$= D^q\{s^\alpha \omega_{n+1}(s)V_n(s)\} = D^q_*\{s^\alpha \omega_{n+1}(s)V_n(s)\}$$
$$= \frac{1}{\Gamma(1-q)} \int_0^s \phi(t)\, t^\alpha (s-t)^{-q} dt, \quad -1 < \alpha, \tag{29}$$

where $\phi(t) := t^{-\alpha}\{t^\alpha\, \omega_{n+1}(t)\, V_n(t)\}'$ is given as follows by using (25)

$$\phi(t) = 8\alpha(t-1)\, U_{n-1}(2t-1)V_n(t) + \omega'_{n+1}(t)V_n(t) + \omega_{n+1}(t)V'_n(t). \tag{30}$$

In (29) the third equality is seen to hold by using in the relation (2) the fact that $t^\alpha \omega_{n+1}(t)V_n(t) = 0$ for $t = 0$. From (29) we have

$$|D^q\{s^\alpha g(s)\} - D^q_n\{s^\alpha g(s)\}| \leq \frac{\max_{0\leq x\leq 1} |\phi(x)|}{\Gamma(1-q)} \int_0^s t^\alpha (s-t)^{-q} dt. \tag{31}$$

The sum in magnitude of the second and last terms in the right hand side of (30) is less than $8nL_n + 2L'_N$, see the proof of Lemma 3.1 in [16]. Further noting that $|U_{n-1}(2t-1)| \leq n$ for $0 \leq t \leq 1$ in (30) we have

$$\max_{0\leq t\leq 1} |\phi(t)| \leq 8n(\alpha+1)L_n + 2L'_n. \tag{32}$$

We see that Lemma 4.1 is established by using above relation (32) and $\int_0^s t^\alpha (s-t)^{-q} dt = s^{\alpha+1-q}\Gamma(\alpha+1)\Gamma(1-q)/\Gamma(\alpha+2-q)$ in (31) and by noting that $\alpha + 1 - q \geq 0$ and $0 \leq s \leq 1$ □.

Theorem 4.2 *Suppose that $g(z)$ is single-valued and analytic inside and on $\mathcal{E}_\rho$ defined by (26) and let $K = \max_{z\in\mathcal{E}_\rho} |g(z)|$. Then the approximation $D^q_n\{s^\alpha g(s)\}$ uniformly converges to $D^q\{s^\alpha g(s)\}$ as $n \to \infty$ as follows,*

$$|D^q\{s^\alpha g(s)\} - D^q_n\{s^\alpha g(s)\}|$$
$$\leq 16K\rho \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+2-q)} \cdot \frac{n(\alpha+1)(\rho-1)^2 + \rho}{(\rho-1)^4\,(\rho^n - \rho^{-n})} = O(n\rho^{-n}),\ \ \rho > 1. \tag{33}$$

Proof. The theorem is established in the same line as the proof of Theorem 3.2 in [16]. □

Since our goal is to construct an automatic quadrature method, we wish to estimate the error of the approximation $D^q_n\{s^\alpha g(s)\}$ (12) in terms of the available coefficients a_k of $p_n(t)$, particularly $|V_n(t)|$ in terms of $|a_k|$. Suppose that $g(z)$ is a meromorphic function which has only simple pole at the point $z = (\beta + \beta^{-1} + 2)/4$ in an ellipse $\mathcal{E}_\sigma$, $1 < \rho < \sigma$, where $1 < \rho < |\beta| < \sigma$. Let $r = |\beta|$, then in the way similar to the (26)∼(30) in [16] we have

$$|D^q\{s^\alpha g(s)\} - D_n^q\{s^\alpha g(s)\}| \le 2\{4n(\alpha+1)L_n + L_n'\}\frac{\Gamma(\alpha+1)}{\Gamma(\alpha+2-q)}$$
$$\sim \frac{8n(\alpha+1)L_n\,\Gamma(\alpha+1)}{\Gamma(\alpha+2-q)} \lesssim \frac{8n\,\Gamma(\alpha+2)\,r\,|a_n|}{\Gamma(\alpha+2-q)\,(r-1)^2} =: E_n(g). \tag{34}$$

Remark 1 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 $D_n^q\{s^\alpha g(s)\}$ converging to $D^q\{s^\alpha g(s)\}$, until a stopping criterion is satisfied. It is an usual and simple way to double the degree n of $p_n(t)$ (4) for generating the sequence $D_n^q\{s^\alpha g(s)\}$ (12), see [7]. 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 $\{p_n\}$ until $E_n(g)$ (34) is less than or equal to the required tolerance ε for $D^q\{s^\alpha g(s)\}$.

5 Numerical examples

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

Table 1
Approximations to $D^{0.1}\{s^{-0.9}/(s+0.05)\}$ with the required tolerance $\varepsilon = 10^{-7}$ for $0 \le s \le 1$. The number $n+1$ of function evaluations required to satisfy ε is 65.

s	approximation	error
0.0005	−376.397867398 *11*	2.2E−10
0.05	−177.52833096 *211*	1.6E−10
0.25	−53.0193366622 *88*	3.3E−11
0.45	−30.2273911052 *81*	3.2E−12
0.85	−15.834374405 *900*	2.3E−12
0.95	−14.101576574655 *3*	1.5E−13

Table 2
Approximations to $D^q(s^{-0.7}\sin as)$, $0 \le s \le 1$. The numbers $n+1$ of function evaluations required to satisfy the tolerances $\varepsilon = 10^{-6}$ 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.

		$\varepsilon = 10^{-6}$		$\varepsilon = 10^{-9}$	
q	a	$n+1$	E_n	$n+1$	E_n
0.1	2.0	11	2.9E−10	17	4.9E−15
	12.0	25	5.4E−12	25	5.4E−12
0.5	2.0	13	2.0E−11	17	7.5E−14
	12.0	25	1.1E−10	33	8.5E−12

Table 3
Approximations to (B1) $D^q\{s^q/(s+a)\}$ and to (B2) $D^q\{s^{q-1}/(s+a)\}$ with the required tolerances $\varepsilon = 10^{-6}$ and 10^{-9}

			$\varepsilon = 10^{-6}$		$\varepsilon = 10^{-9}$	
	q	a	$n+1$	E_n	$n+1$	E_n
(B1)	0.1	0.05	65	1.2E−11	81	5.8E−14
		0.5	21	1.5E−11	25	8.8E−14
	0.5	0.05	65	3.8E−11	81	1.4E−13
		0.5	21	3.6E−11	25	2.8E−13
(B2)	0.1	0.05	65	3.9E−9	81	5.5E−11
		0.5	21	6.0E−10	25	8.3E−12
	0.5	0.05	65	3.5E−9	81	4.7E−11
		0.5	21	5.4E−10	25	7.5E−12

We compute the following test problems (A)∼(D) with exact values in the right hand sides,

$$\text{(A)}\ D^q(s^\alpha \sin as) = D^q\{s^{\alpha+1} a \sum_{k=0}^{\infty}(-1)^k (as)^{2k}/(2k+1)!\}$$

$$= s^{\alpha+1-q} a \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(\alpha+2k+2)\,(as)^{2k}}{(2k+1)!\,\Gamma(\alpha+2k+2-q)},$$

$$q = 0.1, 0.5, \quad \alpha = -0.7, \quad a = 2, 12,$$

$$\text{(B1)}\ D^q\Big(\frac{s^q}{s+a}\Big) = \frac{a^q\Gamma(q+1)}{(s+a)^{q+1}}, \qquad \text{(B2)}\ D^q\Big(\frac{s^{q-1}}{s+a}\Big) = -\frac{a^{q-1}\,\Gamma(q+1)}{(s+a)^{q+1}},$$

$$q = 0.1, 0.5, \quad a = 0.05, 0.5,$$

Table 4
Approximations to (C1) $D^q\{s^q/(s^2+a^2)\}$ and to (C2) $D^q\{s^{q-1}/(s^2+a^2)\}$ with the required tolerances $\varepsilon = 10^{-6}$ and 10^{-9}

	q	a	$\varepsilon = 10^{-6}$ $n+1$	$\varepsilon = 10^{-6}$ E_n	$\varepsilon = 10^{-9}$ $n+1$	$\varepsilon = 10^{-9}$ E_n
(C1)	0.1	0.05	81	1.5E−8	129	1.1E−12
		0.5	21	7.4E−9	33	7.3E−15
	0.5	0.05	97	1.3E−10	129	4.3E−12
		0.5	25	4.2E−10	33	2.9E−14
(C2)	0.1	0.05	81	1.0E−6	129	2.2E−10
		0.5	21	2.2E−7	33	4.8E−13
	0.5	0.05	97	1.1E−8	129	1.6E−10
		0.5	25	6.1E−9	33	4.3E−13

$$\text{(C1)}\ D^q\Big(\frac{s^q}{s^2+a^2}\Big) = \frac{a^{q-1}\Gamma(q+1)}{(s^2+a^2)^{(q+1)/2}} \cos\{(q+1)\arctan\frac{s}{a}\},$$

$$\text{(C2)}\ D^q\Big(\frac{s^{q-1}}{s^2+a^2}\Big) = -\frac{a^{q-2}\,\Gamma(q+1)}{(s^2+a^2)^{(q+1)/2}} \sin\{(q+1)\arctan\frac{s}{a}\},$$

$$q = 0.1, 0.5, \quad a = 0.05, 0.5,$$

$$\text{(D)}\ D^{1/2}\{s^{1/4}J_{1/2}(2\sqrt{s})\} = D^{1/2}[s^{1/2}\cdot\{s^{-1/4}J_{1/2}(2\sqrt{s})\}] = J_0(2\sqrt{s}).$$

Table 1 shows the approximations $D_n^{0.1}\{s^{-0.9}/(s+0.05)\}$ and actual errors $|D^{0.1}\{s^{-0.9}/(s+0.05)\} - D_n^{0.1}\{s^{-0.9}/(s+0.05)\}|$ with the required tolerance $\varepsilon = 10^{-7}$ for various values of $s \in (0,1)$. The number $n+1$ of function evaluations required is 65. 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 $\varepsilon = 10^{-6}$ and 10^{-9} and the actual maximum errors E_n defined by

$$E_n = \max_{1\le j\le m} |D^q f(s_j) - D_n^q f(s_j)|, \quad s_j = (j-0.5)/m, \quad j = 1, 2, \dots, m,$$

where $f(s) = s^\alpha g(s)$ and we choose large m, say, $m = 2000$. Tables 3∼4 show the results for the problems (B)∼(C), respectively. For the problem (D) including the Bessel function $J_{1/2}(2\sqrt{s})$ we choose $f(s) = s^{1/2}g(s)$ where $g(s)$ is a smooth function [17, p.227] given by

$$g(s) = s^{-1/4}J_{1/2}(2\sqrt{s}) = \sum_{k=0}^{\infty} \frac{(-s)^k}{\Gamma(k+1.5)\,k!}.$$

Then the problem is very easy to approximate, indeed $n+1 = 9$ for the tolerance $\varepsilon = 10^{-9}$ with $E_n = 1.2 \times 10^{-15}$.

From Tables 2∼4 we see that the present automatic method could approximate successfully the fractional derivatives (A)∼(C) with varied values of q and a as well as $s \in [0, 1]$ for functions $f(s) = s^\alpha g(s)$ where $\alpha \geq q-1$ and $g(s)$ are well-behaved functions. The present scheme could give an uniform approximation to $D^q\{s^\alpha g(s)\}$, namely a set of approximations for various values of s satisfying the required tolerance ε.

It appears that we have no other automatic methods to be compared in performance with the present method although some computational schemes exist. One of the remaining problems is to approximate fractional derivatives with a non-integer q such that $1 \leq m < q < m+1$ for a positive integer m, namely $\frac{d^m}{ds^m} D^{q-m}\{s^\alpha g(s)\}$, $\alpha > -1$.

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