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DISCRETIZED FRACTIONAL CALCULUS*

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Abstract. For the numerical approximation of fractional integrals

$$I^{\alpha}f(x)=\frac{1}{\Gamma(\alpha)}\int_0^x (x-s)^{\alpha-1}f(s)\,ds \qquad (x\geqq 0)$$

with $f(x)=x^{\beta-1}g(x)$, g smooth, we study convolution quadratures. Here approximations to $I^{\alpha}f(x)$ on the grid $x=0,h,2h,\cdots,Nh$ are obtained from a discrete convolution with the values of f on the same grid. With the appropriate definitions, it is shown that such a method is convergent of order p if and only if it is stable and consistent of order p. We introduce fractional linear multistep methods: The αth power of a pth order linear multistep method gives a pth order convolution quadrature for the approximation of I^{α}. The paper closes with numerical examples and applications to Abel integral equations, to diffusion problems and to the computation of special functions.

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1. Introduction. Fractional calculus is an area having a long history whose infancy dates back to the beginnings of classical calculus, and it is an area having interesting applications. The numerical approximation of the objects of classical calculus, i.e., integrals and derivatives, has for a long time been a standard topic in numerical analysis. However, the state of the art is far less advanced for fractional integrals. Hopefully, the present work contributes to narrow this gap.

Very readable introductions to fractional calculus are given by Lavoie, Osler and Tremblay [12] and by Riesz [19]. See also the book of Oldham and Spanier [18] which contains many references and applications from different areas such as special functions of mathematical physics and diffusion equations. For easy reference we collect first some basic definitions and results.

We consider *Abel–Liouville integrals* of order α (often also called Riemann–Liouville integrals),

$$I^{\alpha}f(x)=\frac{1}{\Gamma(\alpha)}\int_0^x (x-s)^{\alpha-1}f(s)\,ds \qquad (x\geqq 0) \quad \text{for } \operatorname{Re}\alpha>0, \tag{1.1}$$

where Γ denotes Euler's gamma function.

$I^{\alpha}f(x)$ depends analytically on α (for fixed f and x). If f is k-times continuously differentiable on $[0,x]$, it can be continued analytically to α with negative real part via

$$I^{\alpha}f(x)=\frac{d^k}{dx^k}I^{\alpha+k}f(x) \quad \text{for } \operatorname{Re}\alpha>-k. \tag{1.2}$$

If $-k\leqq \operatorname{Re}\alpha<0$ and $f^{(j)}(0)=0$ for $j=0,1,\cdots,k-1$, then $y(x)=I^{\alpha}f(x)$ is the solution of the first-kind *Abel integral equation*

$$\frac{1}{\Gamma(-\alpha)}\int_0^x (x-s)^{-\alpha-1}y(s)\,ds=f(x) \qquad (x\geqq 0). \tag{1.3}$$

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For integer α, I^α is simply repeated integration or differentiation:

$$I^k f(x) = \int_0^x \int_0^{x_k} \cdots \int_0^{x_2} f(x_1)\,dx_1\,dx_2 \cdots dx_k,$$
$$I^0 f(x) = f(x),$$
$$I^{-k} f(x) = \frac{d^k}{dx^k} f(x).$$

I^α is therefore often called *fractional integral* of order α and also denoted $D^{-\alpha}$, the *fractional derivative* of order $-\alpha$.

We extend the definition to functions $f(x) = x^{\beta-1} g(x)$, where g is sufficiently differentiable for $x \geqq 0$ and $\beta \neq 0, -1, -2, \cdots$ is arbitrary. The relation

$$\left(I^\alpha \frac{t^{\beta-1}}{\Gamma(\beta)} \right)(x) = \frac{x^{\alpha+\beta-1}}{\Gamma(\alpha+\beta)} \qquad (\operatorname{Re}\alpha > 0, \operatorname{Re}\beta > 0) \tag{1.4}$$

can be used as a definition for general $\alpha, \beta \in \mathbb{C}$, $\beta \neq 0, -1, -2, \cdots$. Expanding g as a Taylor series with Bernoulli remainder we see that $(I^\alpha t^{\beta-1} g)(x)$ is then well defined.

For the numerical approximation we wish to preserve two characteristic properties of I^α:

(i) the homogeneity of I^α

$$(I^\alpha f)(x) = x^\alpha (I^\alpha f(tx))(1);$$

(ii) the convolution structure of I^α

$$I^\alpha f = \frac{1}{\Gamma(\alpha)} t^{\alpha-1} * f.$$

So we consider *convolution quadratures*

$$I_h^\alpha f(x) = h^\alpha \sum_{j=0}^{n} \omega_{n-j} f(jh) + h^\alpha \sum_{j=0}^{s} w_{nj} f(jh) \qquad (x = nh) \tag{1.5}$$

where the convolution quadrature weights ω_n $(n \geqq 0)$ and the starting quadrature weights w_{nj} $(n \geqq 0, j = 0, \cdots, s;$ s fixed) do not depend on h.

Because of the factor h^α we have then the homogeneity relation

$$(I_h^\alpha f)(x) = x^\alpha \big(I_{h/x}^\alpha f(tx) \big)(1).$$

Also the convolution structure is essentially preserved. It is violated only by the few correction terms of the starting quadrature which will be necessary for high order schemes. For the computation of the values $I_h^\alpha f(nh)$ $(n = 0, \cdots, N-1)$ one needs only N evaluations of the function f and, using fast Fourier transform techniques, only $O(N \log N)$ additions and multiplications.

There remains the important question: How have the weights ω_n and w_{nj} to be chosen in order that $I_h^\alpha f(x)$ approximate $I^\alpha f(x)$ with a prescribed order $O(h^p)$? A complete answer is given in §2. After introducing the appropriate definitions we show in Theorem 2.5 that a convolution quadrature is convergent of order p if and only if it is stable and consistent of order p. This result is an extension of Dahlquist's [3] classical theorem on linear multistep methods. An easy way of computing a convolution quadrature of order p is by using a pth order linear multistep method to the power α (Theorem 2.6), called a fractional linear multistep method. The proofs of the results in §2 constitute §3. In §4 we give some brief remarks on the implementation of fractional linear multistep methods. §5 contains numerical examples for some applications of fractional calculus: Abel's integral equation, diffusion in a half-space, special functions of mathematical physics.

We conclude this section with a remark on the notation: If a function $f(x)$ is undefined for $x=0$, we put for simplicity $f(0)=0$. The convolution of two functions $f(x)$, $g(x)$ defined on $x\geqq 0$ is denoted by

$$(f*g)(x)=\int_0^x f(x-s)g(s)\,ds \qquad (x\geqq 0).$$

Given a sequence $a=(a_n)_0^\infty$ we denote by

$$a(\zeta)=\sum_{n=0}^{\infty} a_n\zeta^n$$

its generating power series. We do not distinguish between a formal power series, a convergent power series and the analytical function with which it coincides in its disc of convergence. We refer to (a_n) as the coefficients of $a(\zeta)$.

2. Convergence of convolution quadratures; fractional linear multistep methods. To motivate the following definitions and results we consider first the case $\alpha=1$ in (1.1) and (1.5).

If a linear multistep method (ρ,σ) (where, as usual, ρ and σ denote the generating polynomials of the method, see e.g. Henrici [8]) is applied to the quadrature problem

$$y'(x)=f(x),\quad y(0)=0,\quad \text{i.e.}\quad y(x)=\int_0^x f(s)\,ds,$$

it is well known [17], [20], [15] that the resulting numerical solution can be written as a convolution quadrature (1.5) where the weights ω_n are the coefficients of

$$\omega(\zeta)=\frac{\sigma(1/\zeta)}{\rho(1/\zeta)}. \tag{2.1}$$

The convergence of a linear multistep method is determined by its stability and consistency (Dahlquist [3], [4], also e.g. in Henrici [8]). In terms of the quadrature weights ω_n, the method is stable if and only if ω_n are bounded. Consistency of order p can be expressed as

$$h\omega(e^{-h})=1+O(h^p).$$

In the following definitions we extend these concepts to arbitrary $\alpha\in\mathbf{C}$. Here $\omega=(\omega_n)_0^\infty$ is a convolution quadrature as in (1.5).

DEFINITION 2.1. A convolution quadrature ω is *stable* (for I^α) if

$$\omega_n=O(n^{\alpha-1}).$$

DEFINITION 2.2. A convolution quadrature ω is *consistent of order* p (for I^α) if

$$h^\alpha\omega(e^{-h})=1+O(h^p).$$

Here and in the following p is a positive integer.

Remark. For $\operatorname{Re}\alpha > 0$ this condition can be interpreted as

$$h^\alpha \sum_{j=0}^{\infty} \omega_j e^{-jh} = \frac{1}{\Gamma(\alpha)} \int_0^\infty t^{\alpha-1} e^{-t}\, dt + O(h^p),$$

that is, ω yields an $O(h^p)$ approximation to the integral of the exponential function on the interval $(0, \infty)$.

For the following it is convenient to introduce the notation

$$\Omega_h^\alpha f(x) = h^\alpha \sum_{j=0}^{n} \omega_{n-j} f(jh) \qquad (x = nh), \tag{2.2}$$

which is the convolution part of (1.5), and

$$E_h^\alpha = \Omega_h^\alpha - I^\alpha, \tag{2.3}$$

the convolution quadrature error.

DEFINITION 2.3. A convolution quadrature ω is *convergent of order* p (to I^α) if

$$\left(E_h^\alpha t^{\beta-1}\right)(1) = O(h^\beta) + O(h^p) \quad \text{for all } \beta \in \mathbb{C}, \beta \neq 0, -1, -2, \cdots. \tag{2.4}$$

This definition is motivated by the following result.

THEOREM 2.4. *Let* ω *satisfy* (2.4). *Then we have*:

(i) *For every* $\beta \neq 0, -1, -2, \cdots$ *there exists a starting quadrature*

$$w_{nj} = O(n^{\alpha-1}) \qquad (n \geqq 0, j = 0, \cdots, s) \tag{2.5}$$

such that for any function

$$f(x) = x^{\beta-1} g(x), \quad g \textit{ sufficiently differentiable}, \tag{2.6}$$

the approximation $I_h^\alpha f$ *given by* (1.5) *satisfies*

$$I_h^\alpha f(x) - I^\alpha f(x) = O(h^p) \tag{2.7}$$

uniformly for $x \in [a, b]$ *with* $0 < a < b < \infty$. (*More precisely, let* $\tilde{\beta} = \beta + k$ (k *integer*) *such that* $0 < \operatorname{Re}\tilde{\beta} \leqq 1$. *Then*

$$I_h^\alpha f(x) - I^\alpha f(x) = O(x^{\alpha+\tilde{\beta}-1} h^p) \textit{ uniformly for bounded } x.) \tag{2.8}$$

(ii) *For every* $\beta \neq 0, -1, -2, \cdots$ *there exists a starting quadrature* w_{nj} (*which does not necessarily satisfy* (2.5)) *such that for any function* (2.6) *the approximation* $I_h^\alpha f$ *satisfies* (2.7) *uniformly for bounded* x.

Remarks. a) Trivially, (i) implies (2.4).

b) The weights w_{nj} are constructed such that $I_h^\alpha t^{q+\beta-1} = I^\alpha t^{q+\beta-1}$ for all integer $q \geqq 0$ with $\operatorname{Re}(q+\beta-1) \leqq p-1$ in (i) and (ii), and additionally those with $\operatorname{Re}(q+\alpha+\beta-1) < p$ in (ii).

c) More generally, for $\beta_1, \cdots, \beta_m$ a starting quadrature (2.5) can be given for functions $f(x) = \sum_{j=1}^m x^{\beta_j - 1} g_j(x)$, g_j sufficiently differentiable, such that (2.7) holds.

In the following we consider convolution quadratures ω for which

$$\omega(\zeta) = r_1(\zeta)^\alpha r_2(\zeta) \tag{2.9}$$

where $r_i(\zeta)$ are rational functions.

We can now give the main result of this paper.

THEOREM 2.5. *A convolution quadrature* (2.9) *is convergent of order p if and only if it is stable and consistent of order p.*

Remark. a) For the special case $\alpha=1$, Theorem 2.5 reduces in essence to Dahlquist's convergence theorem for linear multistep methods [3], [4].

b) As the proof shows, condition (2.9) can be considerably relaxed. However, the class (2.9) is probably large enough for all practical applications.

For $\alpha=k$ a positive integer, $I^k f = II\cdots I\, f$ (k-times) is simply the repeated integral of f. If we take $I_h f$ to be the solution of a linear multistep method (ρ,σ) applied to $y'=f$, $y(0)=0$ (so that $y=If$), then the repeated method $I_h^k f = I_h \cdots I_h f$ can be rewritten as a convolution quadrature (1.5) where the weights are the coefficients of the power series $\omega(\zeta)^k$, with $\omega(\zeta)$ given by (2.1). This can be interpreted as the kth power of the multistep method. We remark that squaring linear multistep methods ($k=2$) has been used in the literature, see e.g. Dahlquist [5] and Jeltsch [10]. The following theorem shows that one can also take fractional powers of linear multistep methods. This result is a corollary of Theorem 2.5. It provides a simple means for constructing convolution quadratures for arbitrary $\alpha\in\mathbb{C}$.

THEOREM 2.6 (fractional linear multistep methods). *Let* (ρ,σ) *denote an implicit linear multistep method which is stable and consistent of order p. Assume that the zeros of* $\sigma(\zeta)$ *have absolute value less than* 1. *Let* $\omega(\zeta)$, *given by* (2.1), *denote the generating power series of the corresponding convolution quadrature* ω. *Define* $\omega^\alpha=(\omega_n^{(\alpha)})_0^\infty$ *by*

$$\omega^\alpha(\zeta)=\omega(\zeta)^\alpha. \tag{2.10}$$

Then the convolution quadrature ω^α *is convergent of order p* (*to* I^α).

We conclude this section with some examples.

Example 2.7. The *fractional Euler method*, $\omega^\alpha(\zeta)=(1-\zeta)^{-\alpha}$, is of historical interest. The method reads

$$I_h^\alpha f(x)=h^\alpha \sum_{0\leq jh\leq x} (-1)^j\binom{-\alpha}{j} f(x-jh). \tag{2.11}$$

For $\alpha=-k$ ($k=1,2,3,\cdots$) this is just the kth backward difference quotient. Starting from this observation, Liouville [14, p. 107] had already introduced fractional derivatives by a formula similar to (2.11). Grünwald [7] and Letnikov [13] have shown that (2.11) converges to the Abel–Liouville integral $I^\alpha f(x)$ (for $\operatorname{Re}\alpha>0$). Their proof (cf. [12, p. 248], [18, p. 51]), however, does not reveal the fact that the method yields an $O(h)$-approximation.

Example 2.8. The $(p+1)$-point backward difference formula (BDF), see e.g. Henrici [8, §5.1-4], is of order p and satisfies for $p\leqq 6$ the assumptions of Theorem 2.6. The *fractional* BDF *methods* given in Table 1 are therefore convergent of order p. For $\alpha=-1$ the method reduces to the usual $(p+1)$-point backward difference quotient.

TABLE 1
Generating functions for $(\text{BDF}p)^\alpha$, $1\leqq p\leqq 6$.

p	$\omega^\alpha(\zeta)$
1	$(1-\zeta)^{-\alpha}$
2	$(3/2-2\zeta+1/2\zeta^2)^{-\alpha}$
3	$(11/6-3\zeta+3/2\zeta^2-1/3\zeta^3)^{-\alpha}$
4	$(25/12-4\zeta+4\zeta^2-4/3\zeta^3+1/4\zeta^4)^{-\alpha}$
5	$(137/60-5\zeta+5\zeta^2-10/3\zeta^3+5/4\zeta^4-1/5\zeta^5)^{-\alpha}$
6	$(147/60-6\zeta+15/2\zeta^2-20/3\zeta^3+15/4\zeta^4-6/5\zeta^5+1/6\zeta^6)^{-\alpha}$

Example 2.9. The *fractional trapezoidal rule*, $\omega^\alpha(\zeta)=(\frac{1}{2}(1+\zeta)/(1-\zeta))^\alpha$, is convergent of order 2 if $\mathrm{Re}\,\alpha\geqq 0$. Since the numerator has a zero on the unit circle, the method is not stable for $\mathrm{Re}\,\alpha<0$ (see (3.9), (3.10)).

Example 2.10. The following class of methods can be interpreted as generalized *Newton–Gregory formulas.*

Let γ_i denote the coefficients of

$$\sum_{i=0}^{\infty}\gamma_i(1-\zeta)^i=\left(\frac{\ln\zeta}{\zeta-1}\right)^{-\alpha}$$

(see Lemma 3.2), and put

$$\omega^\alpha(\zeta)=(1-\zeta)^{-\alpha}\left[\gamma_0+\gamma_1(1-\zeta)+\cdots+\gamma_{p-1}(1-\zeta)^{p-1}\right].$$

Then ω^α is convergent of order p (to I^α). For $\alpha=1$ this method reduces to the pth order Newton–Gregory formula (i.e. implicit Adams method), for $\alpha=-1$ to the $(p+1)$-point backward difference quotient.

3. Proofs. We give first the proof of the central result, Theorem 2.5, and of its corollary, Theorem 2.6, and finally the proof of Theorem 2.4. We begin with some preparations.

Preparations. We shall repeatedly make use of the following asymptotic expansion for binomial coefficients (cf. [6, p. 47])

$$(3.1)\quad (-1)^n\binom{-\alpha}{n}=\frac{n^{\alpha-1}}{\Gamma(\alpha)}\left[1+a_1n^{-1}+a_2n^{-2}+\cdots+a_{N-1}n^{-(N-1)}+O(n^{-N})\right]$$

where the coefficients a_j depend analytically on α. $\Omega_h^\alpha f(x)$, introduced in (2.2), can be extended to

$$\Omega_h^\alpha f(x)=h^\alpha\sum_{0\leqq jh\leqq x}\omega_j f(x-jh)\qquad(x\geqq 0),$$

which is the convolution of the sequence $h^\alpha\omega$ with f. Therefore Ω_h^α commutes with convolution

$$\Omega_h^\alpha(f*g)=(\Omega_h^\alpha f)*g,$$

if f is continuous and g is locally integrable.

This property is often shared by I^α:

$$I^\alpha(f*g)=(I^\alpha f)*g$$

which holds for locally integrable g and continuous f if $\mathrm{Re}\,\alpha>0$, and also for f with $f^{(j)}(0)=0$ $(j=0,\cdots,k-1)$ if $\mathrm{Re}\,\alpha>-k$. In this case also the convolution quadrature error $E_h^\alpha=\Omega_h^\alpha-I^\alpha$ satisfies

$$(3.2)\qquad E_h^\alpha(f*g)=(E_h^\alpha f)*g.$$

The proof of the above statements is easy and therefore omitted.

The homogeneity of I^α and $t^{\beta-1}$ yields

$$(3.3)\qquad \left(E_h^\alpha t^{\beta-1}\right)(x)=x^{\alpha+\beta-1}\left(E_{h/x}^\alpha t^{\beta-1}\right)(1).$$

Formulas (3.1)–(3.3) and an analytic continuation argument will be the essential tools in the proof of Theorem 2.5.

Proof of Theorem 2.5. We break the proof into several steps which are formulated as lemmas.

LEMMA 3.1. *If* $(E_h^\alpha t^{k-1})(1)=O(h^k)+O(h^p)$ *for* $k=1,2,3,\cdots$, *then* ω *is consistent of order* p.

In particular, convergence of order p implies consistency of order p.

Proof. We look first at the quadrature error for e^{t-x} (as a function of t) on the interval $[0,x]$,

$$e_h(x)=\left(E_h^\alpha e^{t-x}\right)(x)=h^\alpha\sum_{0\leqq jh\leqq x}\omega_j e^{-jh}-\left(I^\alpha e^{t-x}\right)(x).$$

As $x\to\infty$, the first expression of the difference tends to $h^\alpha\omega(e^{-h})$, and

$$\left(I^\alpha e^{t-x}\right)(x)\to 1\qquad(x\to\infty).$$

(For $\operatorname{Re}\alpha>0$ this is immediate from the definition of Euler's gamma function. For $\operatorname{Re}\alpha\leqq 0$ it follows in the same way as in the derivation of (3.5) below, with E_h^α replaced by I^α). So we have

$$e_h(\infty)=h^\alpha\omega(e^{-h})-1. \tag{3.4}$$

We expand e^{t-x} at $t=0$,

$$e^{t-x}=\sum_{k=0}^{q}\frac{t^k}{k!}e^{-x}+\frac{1}{q!}\left(\tau^q * e^{\tau-x}\right)(t),$$

with $q+1\geqq\max\{p,p-\operatorname{Re}\alpha\}$. We write

$$e_h(x)=e_h^1(x)+e_h^2(x)$$

with

$$e_h^1(x)=e^{-x}\sum_{k=0}^{q}\frac{1}{k!}\left(E_h^\alpha t^k\right)(x).$$

By (3.3), $(E_h^\alpha t^k)(x)$ has only polynomial growth as $x\to\infty$. Hence

$$e_h^1(\infty)=0.$$

By (3.2),

$$e_h^2(x)=\frac{1}{q!}E_h^\alpha\left(t^q * e^{t-x}\right)(x)=\frac{1}{q!}\left(\left(E_h^\alpha t^q\right) * e^{t-x}\right)(x)$$
$$=\frac{1}{q!}\int_0^x e^{-s}\left(E_h^\alpha t^q\right)(s)\,ds.$$

So we obtain

$$e_h(\infty)=\frac{1}{q!}\int_0^\infty e^{-s}\left(E_h^\alpha t^q\right)(s)\,ds. \tag{3.5}$$

By (3.3) and by assumption,

$$\left(E_h^\alpha t^q\right)(s)=s^{q+\alpha}\left(E_{h/s}^\alpha t^q\right)(1)=O\left(s^{q+\alpha-p}h^p\right).$$

From (3.4) and (3.5) we obtain hence

$$h^{\alpha}\omega(e^{-h})-1=O(h^{p}),$$

i.e., consistency of order p. □

Our next aim is to give in Lemma 3.2 a characterization of consistency. We may write

$$\omega(\zeta)=(1-\zeta)^{-\mu}\tilde{\omega}(\zeta)$$

where μ is chosen such that $\tilde{\omega}(\zeta)$ is holomorphic at 1 and $\tilde{\omega}(1)\neq 0$.

Consistency implies immediately $\mu=\alpha$ and $\tilde{\omega}(1)=1$. We expand $\omega(\zeta)$ at 1:

$$\begin{aligned}(3.6)\qquad \omega(\zeta)=(1-\zeta)^{-\alpha}\Big[c_0+c_1(1-\zeta)+c_2(1-\zeta)^2+\cdots \\ +c_{N-1}(1-\zeta)^{N-1}+(1-\zeta)^{N}\tilde{r}(\zeta)\Big]\end{aligned}$$

where $\tilde{r}(\zeta)$ is holomorphic at 1.

We can characterize consistency in terms of the coefficients c_i.

LEMMA 3.2. *Let γ_i denote the coefficients of $\sum_0^\infty \gamma_i(1-\zeta)^i=(-\ln\zeta/(1-\zeta))^{-\alpha}$. Then*

ω is consistent of order p

if and only if the coefficients c_i in (3.6) *satisfy*

$$c_i=\gamma_i \quad \textit{for} \quad i=0,1,\cdots,p-1.$$

Proof. The expression

$$h^{\alpha}\omega(e^{-h})=\left(\frac{h}{1-e^{-h}}\right)^{\alpha}\tilde{\omega}(e^{-h})$$

is $1+O(h^p)$ if and only if

$$\tilde{\omega}(e^{-h})=\left(\frac{h}{1-e^{-h}}\right)^{-\alpha}+O(h^p),$$

which holds if and only if

$$\tilde{\omega}(\zeta)=\left(\frac{-\ln\zeta}{1-\zeta}\right)^{-\alpha}+O((1-\zeta)^p). \qquad \square$$

Whether the method ω is stable depends on the remainder in the expansion (3.6). We rewrite (3.6) as

$$(3.7)\quad \omega(\zeta)=(1-\zeta)^{-\alpha}\Big[c_0+c_1(1-\zeta)+\cdots+c_{N-1}(1-\zeta)^{N-1}\Big]+(1-\zeta)^{N}r(\zeta)$$

where $r(\zeta)=(1-\zeta)^{-\alpha}\tilde{r}(\zeta)$.

LEMMA 3.3. *ω is stable if and only if the coefficients r_n of $r(\zeta)$ in* (3.7) *satisfy*

$$(3.8)\qquad r_n=O(n^{\alpha-1}).$$

Proof. It is immediate from (3.1) that (3.8) implies $\omega_n=O(n^{\alpha-1})$. Conversely, let ω be stable. Then $\omega(\zeta)$ has no singularities in the interior of the unit disc, $|\zeta|<1$, and by (2.9) can therefore be written as

$$(3.9)\qquad \omega(\zeta)=u(\zeta)\prod_{j=0}^{m}(\zeta-\zeta_j)^{-\alpha_j}$$

where the ζ_j are distinct numbers of absolute value 1 (let $\zeta_0=1,\alpha_0=\alpha$), $u(\zeta)$ is holomorphic in a neighbourhood of $|\zeta|\leqq 1$, and $u(\zeta_j)\neq 0$, $\alpha_j\neq 0,-1,-2,\cdots$. Expanding $\omega(\zeta)$ at ζ_j yields (cf. partial fraction decomposition)

$$\omega(\zeta)=\sum_{j=0}^{m}(\zeta-\zeta_j)^{-\alpha_j}p_j(\zeta-\zeta_j)+q(\zeta)$$

where p_j are polynomials, $p_j(0)\neq 0$, and $q(\zeta)$ is analytic in the interior of the unit disc and sufficiently differentiable (say, k-times) on the unit circle $|\zeta|=1$, so that its coefficients are $O(n^{-k})$, (e.g. [11, p. 24]).

It is now seen from (3.1) that

$$\omega_n=O(n^{\alpha-1}) \quad \text{if and only if } \operatorname{Re}\alpha_j\leqq \operatorname{Re}\alpha \text{ for all } j. \tag{3.10}$$

Correspondingly, $r(\zeta)$ can be represented as

$$r(\zeta)=\sum_{j=0}^{m}(\zeta-\zeta_j)^{-\alpha_j}\tilde{p}_j(\zeta-\zeta_j)+\tilde{q}(\zeta)$$

with $\tilde{p}_j$ and $\tilde{q}$ as p_j and q above.

Hence (3.10) holds also with r_n instead of ω_n. This gives (3.8). □

The trivial direction of Lemma 3.3 is used in the next lemma.

LEMMA 3.4. *Convergence implies stability.*

Proof. If ω is convergent, then it is consistent by Lemma 3.1. With $N=1$ in (3.7) we have therefore

$$\omega(\zeta)=(1-\zeta)^{-\alpha}+(1-\zeta)r(\zeta).$$

We study

$$(E_h^\alpha 1)(1)=h^\alpha\sum_{j=0}^{n}\omega_{n-j}-\frac{1}{\Gamma(\alpha+1)} \qquad (hn=1).$$

$\sum_{j=0}^{n}\omega_{n-j}$ is the nth coefficient of

$$\frac{\omega(\zeta)}{1-\zeta}=(1-\zeta)^{-\alpha-1}+r(\zeta).$$

By (3.1) we have

$$(E_h^\alpha 1)(1)=h^\alpha\left[\frac{n^\alpha}{\Gamma(\alpha+1)}+O(n^{\alpha-1})\right]+h^\alpha r_n-\frac{1}{\Gamma(\alpha+1)}=O(h)+h^\alpha r_n \qquad (hn=1)$$

which is $O(h)$ only if $r_n=O(n^{\alpha-1})$. Now Lemma 3.3 completes the proof. □

It remains to show that stability and consistency imply convergence. Let us first have a closer look at the structure of the error.

LEMMA 3.5. *Let $\alpha,\beta\in\mathbb{C}$, $\beta\neq 0,-1,-2,\cdots$. If ω is stable, then the convolution quadrature error of $t^{\beta-1}$ has an asymptotic expansion of the form*

$$(E_h^\alpha t^{\beta-1})(1)=e_0+e_1h+\cdots+e_{N-1}h^{N-1}+O(h^N)+O(h^\beta) \tag{3.11}$$

where the coefficients $e_j=e_j(\alpha,\beta,c_0,\cdots,c_j)$ depend analytically on α, β and the coefficients $c_0,\cdots,c_j$ of (3.7).

Proof. a) We need the following auxiliary result: The convolution of two sequences $u_n = O(n^\mu)$ and $v_n = O(n^\nu)$ with $\nu < \min\{-1, \mu - 1\}$ satisfies

$$\sum_{j=0}^{n} u_{n-j} v_j = O(n^\mu). \tag{3.12}$$

This is seen from

$$\left| \sum_{j=0}^{n} u_{n-j} v_j \right| \leqq |u_n v_0| + |u_0 v_n| + M n^\mu \sum_{j=1}^{n-1} \left(1 - \frac{j}{n}\right)^\mu j^\nu$$

and

$$\left(1 - \frac{j}{n}\right)^\mu \leqq \begin{cases} 1 & \text{if } \mu \geqq 0 \\ (j+1)^{-\mu} & \text{if } \mu < 0 \end{cases} \quad \text{for } 1 \leqq j \leqq n-1.$$

b) For $\beta \neq 0, -1, -2, \cdots$ we obtain from (3.1) an asymptotic expansion

$$\begin{aligned} n^{\beta-1} = b_0(-1)^n \binom{-\beta}{n} + b_1(-1)^n \binom{-\beta+1}{n} + \cdots \\ + b_{N-1}(-1)^n \binom{-\beta+N-1}{n} + O(n^{\beta-1-N}). \end{aligned} \tag{3.13}$$

So we have

$$\begin{aligned} b(\zeta) := \sum_{n=1}^{\infty} n^{\beta-1} \zeta^n = b_0(1-\zeta)^{-\beta} + b_1(1-\zeta)^{-\beta+1} + \cdots \\ + b_{N-1}(1-\zeta)^{-\beta+N-1} + s(\zeta) \end{aligned}$$

where the coefficients s_n of $s(\zeta)$ satisfy

$$s_n = O(n^{\beta-1-N}). \tag{3.14}$$

c) We have to study the expression

$$h^\alpha \sum_{j=1}^{n} \omega_{n-j} (jh)^{\beta-1} \qquad (hn = 1).$$

$y_n = \sum_{j=1}^{n} \omega_{n-j} j^{\beta-1}$ is the nth coefficient of $y(\zeta) = \omega(\zeta) b(\zeta)$ which by inserting (3.7) and (3.13) can be written as

$$\begin{aligned} y(\zeta) = d_0(1-\zeta)^{-(\alpha+\beta)} + d_1(1-\zeta)^{-(\alpha+\beta)+1} + \cdots + d_{2N-2}(1-\zeta)^{-(\alpha+\beta)+2N-2} \\ + \omega(\zeta)s(\zeta) + [b(\zeta) - s(\zeta)](1-\zeta)^N r(\zeta) \end{aligned}$$

where $d_k = \sum_{j=0}^{k} b_{k-j} c_j$.

If N is chosen sufficiently large, then the coefficients of $\omega(\zeta)s(\zeta)$ and

$$[b(\zeta) - s(\zeta)](1-\zeta)^N r(\zeta) = \left[b_0(1-\zeta)^{-\beta+N} + \cdots + b_{N-1}(1-\zeta)^{-\beta+2N-1}\right] r(\zeta)$$

are $O(n^{\alpha-1})$ by (3.1), (3.8), (3.14) and (3.12).

By (3.1) we have therefore

$$y_n = \tilde{e}_0 n^{\alpha+\beta-1} + e_1 n^{(\alpha+\beta-1)-1} + \cdots + e_N n^{(\alpha+\beta-1)-N} + O(n^{\alpha-1}).$$

This gives the desired result for

$$\left(E_h^\alpha t^{\beta-1}\right)(1)=h^{\alpha+\beta-1}y_n-\left(I^\alpha t^{\beta-1}\right)(1) \qquad (hn=1). \qquad \square$$

In Lemma 3.8 below we shall show that $e_0=\cdots=e_{p-1}=0$ if the method is stable and consistent of order p. First, we need two auxiliary results in which we restrict our attention to $\operatorname{Re}\alpha>0$.

LEMMA 3.6. *Let* $\operatorname{Re}\alpha>0$.

If $\left(E_h^\alpha t^{p-1}\right)(1)=O(h^p)$, *then* $\left(E_h^\alpha t^{\beta-1}\right)(1)=O(h^p)$ *for all* $\operatorname{Re}\beta>p$.

Proof. Let $\beta=p+\mu$. By (1.4),

$$t^{\beta-1}=\frac{\Gamma(p+\mu)}{\Gamma(p)\Gamma(\mu)}t^{p-1}*t^{\mu-1}.$$

By (3.3),

$$\left(E_h^\alpha t^{p-1}\right)(x)=O(x^{\alpha-1}h^p).$$

By (3.2),

$$E_h^\alpha\left(t^{p-1}*t^{\mu-1}\right)(1)=\left(E_h^\alpha t^{p-1}*t^{\mu-1}\right)(1)=O(h^p).$$

Hence also

$$\left(E_h^\alpha t^{\beta-1}\right)(1)=O(h^p). \qquad \square$$

Remark. $E_h^\alpha t^{p-1}$ is the Peano kernel of the quadrature ω.

LEMMA 3.7. *Let* $\operatorname{Re}\alpha>0$. *There exist numbers* $\tilde\gamma_0,\tilde\gamma_1,\tilde\gamma_2,\cdots$ (*independent of* ω) *such that the following equivalence holds for stable* ω:

$$\left(E_h^\alpha t^{q-1}\right)(1)=O(h^q) \quad \textit{for } q=1,2,\cdots,p \tag{3.15}$$

if and only if the coefficients c_i *of* (3.7) *satisfy*

$$c_i=\tilde\gamma_i \quad \textit{for } i=0,1,\cdots,p-1. \tag{3.16}$$

Proof. The proof proceeds by induction on p. Trivially the statement holds for $p=0$.

Assume now that Lemma 3.7 has already been proved up to order p. We shall prove it for $p+1$.

Let either of (3.15) or (3.16) hold. By the induction hypothesis, it suffices to show that c_p can be uniquely chosen such that

$$\left(E_h^\alpha t^p\right)(1)=O(h^{p+1}).$$

From Lemma 3.6 (and from Lemma 3.5 for $p=0$) we know already

$$\left(E_h^\alpha t^p\right)(1)=O(h^p). \tag{3.17}$$

For any integer n we may write

$$n^p=\sum_{k=1}^{p+1}b_k\binom{n+k-1}{n}=\sum_{k=1}^{p+1}b_k(-1)^n\binom{-k}{n}$$

so that (with $hn=1$)

$$\left(\Omega_h^\alpha t^p\right)(1)=h^\alpha\sum_{j=0}^n\omega_j(n-j)^p h^p=h^{p+\alpha}\sum_{k=1}^{p+1}b_k\sum_{j=0}^n\omega_j(-1)^{n-j}\binom{-k}{n-j}.$$

The inner sum is the nth coefficient of

$$\frac{\omega(\zeta)}{(1-\zeta)^k}=\tilde{\gamma}_0(1-\zeta)^{-\alpha-k}+\cdots+\tilde{\gamma}_{p-1}(1-\zeta)^{-\alpha+p-1-k}$$
$$+c_p(1-\zeta)^{-\alpha+p-k}+(1-\zeta)^{p+1-k}r(\zeta).$$

Using (3.1), (3.8) and (3.17) we obtain

$$(E_h^\alpha t^p)(1)=\frac{c_p-\tilde{\gamma}_p}{\Gamma(\alpha+1)}h^p+O(h^{p+1})$$

where $\tilde{\gamma}_p$ depends only on α and $\tilde{\gamma}_0,\cdots,\tilde{\gamma}_{p-1}$. Hence (3.15) holds for $p+1$ instead of p if and only if additionally $c_p=\tilde{\gamma}_p$. □

We have now arrived at the final step of the proof.

LEMMA 3.8. *Let $\alpha\in\mathbb{C}$. If ω is stable and consistent of order p, then it is also convergent of order p.*

Proof. Let first $\operatorname{Re}\alpha>0$. Since (3.15) implies consistency of order p by Lemma 3.1, the numbers $\tilde{\gamma}_i$ of Lemma 3.7 and $\gamma_i=\gamma_i(\alpha)$ of Lemma 3.2 are identical.

By Lemmas 3.5 and 3.6 we have then for $\operatorname{Re}\alpha>0$, $\operatorname{Re}\beta>p$

$$e_j\big(\alpha,\beta,\gamma_0(\alpha),\cdots,\gamma_j(\alpha)\big)=0 \qquad (j=0,\cdots,p-1).$$

By analyticity, this holds then for *all* α, β.

If the method is consistent of order p, we have by Lemma 3.2 $c_i=\gamma_i(\alpha)$ for $i=0,\cdots,p-1$. Now Lemma 3.5 gives the result. □

We have thus completed the proof of Theorem 2.5. □

Proof of Theorem 2.6. The linear multistep method is consistent of order p, i.e.

$$h\omega(e^{-h})=1+O(h^p).$$

Taking this relation to power α yields

$$h^\alpha\omega^\alpha(e^{-h})=1+O(h^p),$$

so that ω^α is consistent of order p for I^α. Under the given assumptions on (ρ,σ) we can write

$$\omega(\zeta)=\frac{\sigma(\zeta^{-1})}{\rho(\zeta^{-1})}=\prod_{i=0}^{r}(1-\zeta_i\zeta)^{-1}v(\zeta)$$

where $v(\zeta)$ is analytic and without zeros in a neighbourhood of $|\zeta|\leq 1$, and ζ_i are the zeros of $\rho(\zeta)$ on the unit circle. Hence

$$\omega^\alpha(\zeta)=\prod_{i=0}^{r}(1-\zeta_i\zeta)^{-\alpha}u(\zeta)$$

where $u(\zeta)=v(\zeta)^\alpha$ is analytic in a neighbourhood of $|\zeta|\leq 1$. By (3.9) and (3.10),

$$\omega_n^{(\alpha)}=O(n^{\alpha-1})$$

so that ω^α is stable. Now Theorem 2.5 completes the proof. □

Proof of Theorem 2.4. The proof is based on a Peano kernel technique similar as in Lemmas 3.1 and 3.6.

(i) Fix $\beta \neq 0, -1, -2, \cdots$. Let the integer m such that

$$\operatorname{Re}(m+\beta-1) \leqq p < \operatorname{Re}(m+\beta).$$

A suitable starting quadrature can be chosen by putting

$$h^\alpha \sum_{j=1}^{m} w_{nj}(jh)^{q+\beta-1} + \left(E_h^\alpha t^{q+\beta-1}\right)(1) = 0 \qquad (q=0,1,\cdots,m-1;\ hn=1). \tag{3.18}$$

This gives a Vandermonde type system of equations for $w_{nj}(j=1,\cdots,m)$,

$$\sum_{j=1}^{m} w_{nj} j^{q+\beta-1} = O(n^{\alpha-1}) \quad \text{by (2.4)}.$$

Hence also

$$w_{nj} = O(n^{\alpha-1}) \tag{3.19}$$

as desired.

Let $f(x) = x^{\beta-1}g(x)$, g sufficiently differentiable. Expanding f as a fractional Taylor series with Bernoulli remainder term gives (let $f^{(\mu)} = I^{-\mu}f$)

$$f(x) = \sum_{q=0}^{N} \frac{f^{(q+\beta-1)}(0)}{\Gamma(q+\beta)} x^{q+\beta-1} + \frac{1}{\Gamma(N+\beta)} \left(t^{N+\beta-1} * f^{(N+\beta)}\right)(x). \tag{3.20}$$

If $\operatorname{Re}(N+\beta-1) > p$, then (3.3) and (2.4) yield

$$\left(E_h^\alpha t^{N+\beta-1}\right)(x) = O\left(x^{N-p+\alpha+\beta-1}h^p\right).$$

If additionally $\operatorname{Re}(N-p+\alpha+\beta) > 0$, then (3.2) and the boundedness of $f^{(N+\beta)}$ give

$$\begin{aligned} E_h^\alpha\left(t^{N+\beta-1} * f^{(N+\beta)}\right)(x) &= \left(E_h^\alpha t^{N+\beta-1} * f^{(N+\beta)}\right)(x) \\ &= O\left(x^{N-p+\alpha+\beta}h^p\right) \end{aligned} \tag{3.21}$$

for bounded x.

By our choice of the starting quadrature ((3.18), (3.19)), by the homogeneity relation (3.3) and by (3.20), (3.21) we have

$$\begin{aligned} I_h^\alpha f(x) - I^\alpha f(x) &= E_h^\alpha f(x) + h^\alpha \sum_{j=1}^{m} w_{nj} f(jh) \\ &= O\left(x^{m-p+\alpha+\beta-1}h^p\right) + \cdots + O\left(x^{N-p+\alpha+\beta-1}h^p\right) + O\left(x^{N-p+\alpha+\beta}h^p\right) \\ &= O\left(x^{m-p+\alpha+\beta-1}h^p\right) \quad \text{uniformly for bounded } x. \end{aligned}$$

This gives (i) of Theorem 2.4 (note $\tilde{\beta} = m-p+\beta$).

(ii) If m is (3.18) is replaced by $l > m$ with $\operatorname{Re}(l-p+\alpha+\beta-1) \geqq 0$, then the corresponding starting quadrature weights satisfy

$$w_{nj} = O\left(n^{l-1-p+\alpha+\beta-1}\right),$$

and the same arguments as above show

$$I_h^\alpha f(x) - I^\alpha f(x) = O(h^p) \quad \text{uniformly for bounded } x. \qquad \square$$

4. Implementation.

4.1. Weights of fractional linear multistep methods ω^α. The coefficients of ω^α, defined by (2.10), are computed most efficiently by Fast Fourier Transform (FFT) techniques for formal power series as described by Henrici [9, §5]. The weights $\omega_0^{(\alpha)},\cdots,\omega_{N-1}^{(\alpha)}$ are thus obtained using only $O(N\log N)$ additions and multiplications.

4.2. Starting quadrature weights w_{nj}. Multiplying (3.18) by $n^{q+\alpha+\beta-1}$ and using (1.4) we obtain

(4.1)
$$\sum_{j=1}^{s} w_{nj} j^{q+\beta-1} = \frac{\Gamma(q+\beta)}{\Gamma(\alpha+q+\beta)} n^{q+\alpha+\beta-1} - \sum_{j=1}^{n} \omega_{n-j} j^{q+\beta-1} \qquad (q=0,\cdots,s-1).$$

Exploiting the convolution structure of the right-hand side, the weights $w_{nj}(n=1,\cdots,N$ and $j=1,\cdots,s)$ can be computed from (4.1) with $O(N \log N)$ operations, using FFT-techniques (cf. [9]).

The starting quadrature of (ii) in Theorem 2.4 can be used on short intervals. If w_{nj} of (ii) do not satisfy (2.5), then they dominate ω_n for large n, and errors in the evaluation of $f(jh)$ $(j=1,\cdots,s)$ are unduly magnified.

(As a marginal note: For large n the right-hand side of (4.1) can be computed only with large relative error, due to cancellation of leading digits. Moreover the Vandermonde system is ill-conditioned for large s. Hence the weights w_{nj} are computed with possibly low accuracy. This does, however, *not* affect the accuracy of the quadrature, since it is only important that (4.1) holds up to machine precision).

4.3. Computation of $\Omega_h^\alpha f$. After $f_j=f(jh)$ have been evaluated, the values of the convolution $\Omega_h^\alpha f(nh)=h^\alpha\sum_{j=1}^n \omega_{n-j} f_j (n=1,\cdots,N)$ can be computed simultaneously by FFT-techniques with only $O(N\log N)$ operations.

5. Applications and numerical examples.

5.1. Abel's integral equation. Historically, the first application of fractional calculus was probably given by Abel in his study of the tautochrone problem ([1], see also [18, p. 183]). This led him to the integral equation

$$\frac{1}{\sqrt{\pi}}\int_0^x (x-s)^{-1/2} y(s)\,ds = f(x),$$

the solution of which he found to be

$$y(x)=I^{-1/2}f(x).$$

For our numerical experiments we have used the $(\mathrm{BDF3})^{-1/2}$ method (third order backward differentiation formula to power $-\frac{1}{2}$, see Example 2.8). We give the results for the function

$$f(x)=\frac{x}{1+x}.$$

The exact solution is then given by (see [18, p. 121])

$$I^{-1/2}\frac{x}{1+x} = \frac{2}{\sqrt{\pi}}\sqrt{x}\,{}_2F_1\left(1,2;\ \frac{3}{2};\ -x\right), \tag{5.1}$$

where ${}_2F_1$ denotes the hypergeometric function. The solution at $x=1$ is $y(1)=0.4579033863$. The numerical results are given in Table 2.

TABLE 2

h	numerical solution	error	error$/h^3$
0.04	0.4579085018	$0.512_{10^{-5}}$	0.0799
0.02	0.4579040377	$0.651_{10^{-6}}$	0.0814
0.01	0.4579034683	$0.820_{10^{-7}}$	0.0820

5.2. Diffusion problems. As a simple example, consider the heat equation in a half-space

$$u_t = u_{xx} \qquad (x>0,\ t>0)$$

with initial condition

$$u(x,0)=0 \qquad (x>0),$$

with boundary conditions

$$u(\infty,t)=0 \qquad (t>0)$$

and either

$$\begin{array}{llll} \text{(i)} & u(0,t)=f(t) & (t>0) & \text{or} \\ \text{(ii)} & u_x(0,t)=g(t) & (t>0) & \text{or} \\ \text{(iii)} & u_x(0,t)=G(u(0,t)) & (t>0). & \end{array}$$

The solution at the surface $x=0$ satisfies (cf. [2, App. 2 to Ch. V])

$$u(0,t) = -\frac{1}{\sqrt{\pi}}\int_0^t (t-s)^{-1/2} u_x(0,s)\,ds \qquad (t>0).$$

For boundary conditions (ii) the surface temperature $u(0,t)$ is thus obtained as $-I^{1/2}g(t)$. For boundary conditions (i) this formula is a first kind Abel integral equation for the surface flux $u_x(0,t)$, which hence equals $-I^{-1/2}f(t)$. In case (iii) we obtain a second kind Abel integral equation for $u(0,t)$. The application of fractional linear multistep methods to such equations is discussed in the author's paper [16]. The solution $u(x,t)$ can be recovered from the surface flux by

$$u(x,t) = -\frac{1}{\sqrt{\pi}}\int_0^t (t-s)^{-1/2}\exp\left(\frac{-x^2}{4(t-s)}\right) u_x(0,s)\,ds.$$

As a numerical example related to (ii), we have used the $(\mathrm{BDF4})^{1/2}$ method (see Example 2.8) to compute

$$I^{1/2}\frac{\sin\sqrt{t}}{\sqrt{\pi}} = \sqrt{t}\,J_1(\sqrt{t}), \tag{5.2}$$

where J_1 denotes the Bessel function (see [18, p. 124]). At $t=1$ the solution is $J_1(1)=0.4400505857449$. The numerical results are given in Table 3.

TABLE 3

h	numerical solution	error	error$/h^4$
0.04	0.4400505854008	$-0.344_{10^{-9}}$	$-0.134_{10^{-3}}$
0.02	0.4400505857240	$-0.209_{10^{-10}}$	$-0.130_{10^{-3}}$
0.01	0.4400505857436	$-0.128_{10^{-11}}$	$-0.127_{10^{-3}}$

5.3. Special functions. The relations (5.1) and (5.2) are special cases of

$$ {}_2F_1(a,b;\,c;\,x)=\frac{\Gamma(c)x^{1-c}}{\Gamma(b)}I^{c-b}\left[x^{b-1}(1-x)^{-a}\right] \quad \text{and} $$

$$ J_\mu(\sqrt{x})=\frac{2}{\sqrt{\pi}}(2\sqrt{x})^{-\mu}I^{\mu-1/2}\sin\sqrt{x}\,. $$

Among the special functions which can be represented as fractional integrals of simpler functions are: hypergeometric functions, confluent and generalized hypergeometric functions, Bessel and Struve functions, Legendre functions, elliptic integrals etc. (see [12], [18]). Convolution quadratures for their computation are particularly effective if one is interested in obtaining many values on a grid simultaneously.

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