Generalized Adams methods for fractional differential equations.

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Abstract. We introduce a new family of fractional convolution quadratures based on generalized Adams methods for the numerical solution of fractional differential equations. We discuss their accuracy and linear stability properties. The boundary loci reported show that, when used as Boundary Value Methods, these schemes overcome the classical order barrier for A-stable methods.

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INTRODUCTION

In this paper we are interested in the numerical solution of fractional differential equations (FDEs) of the type

$$D_0^\alpha y(t) = f(t, y(t)), \quad 0 < t \le T, \quad 0 < \alpha < 1, \tag{1}$$

where $D_0^\alpha y(t)$ denotes the Caputo's fractional derivatives defined as [3]

$$D_0^\alpha y(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{y'(u)}{(t-u)^\alpha} du.$$

As well known, the use of the Caputo's definition allows to treat the initial conditions at $t = 0$ for fractional differential equations in the same manner as for integer-order differential equations, whereas this is not possible using the Riemann-Liouville approach (see e.g. [8] for a wide background). Setting $y(0) = y_0$ the solution of (1) exists and is unique under the hypothesis that f is continuous and fulfils a Lipschitz condition with respect to the second variable (see e.g. [4] for a proof). The solution $y(t)$ solves

$$y(t) = y_0 + \frac{1}{\Gamma(\alpha)} \int_0^t (t-u)^{\alpha-1} f(u, y(u)) du, \tag{2}$$

that represents a Volterra integral equation of the second kind with a weakly singular kernel and constant forcing function.
For the numerical solution of (2) we consider the application of *fractional convolution quadratures*. When used over an assigned uniform partition of the interval of integration $I = [0, T]$, given by

$$t_n = nh, \qquad n = 0, 1, \ldots, N, \qquad h = T/N, \tag{3}$$

these schemes provide a discrete problem of the following form

$$y_n = y_0 + h^\alpha \sum_{j=0}^{M} w_{n,j} f_j + h^\alpha \sum_{j=0}^{n+k_2} \omega_{n-j} f_j, \qquad n = M+1, \ldots, N-k_2, \tag{4}$$

where $y_n \approx y(t_n)$, $f_n = f(t_n, y_n)$, the weights $w_{n,j}$ and ω_n are independent of h, and M depends on the order of the method and on α. The terms

$$S_n = y_0 + h^\alpha \sum_{j=0}^{M} w_{n,j} f_j, \qquad \Omega_n = h^\alpha \sum_{j=0}^{n+k_2} \omega_{n-j} f_j$$

are usually called the *starting* and the *convolution* terms, respectively. A convolution quadrature arise, for example, when the integral in (2) is approximated by an Adams product quadrature rule or a fractional linear multistep method [2, 5, 6, 7]. In both cases k_2 is set equal to zero and the resulting schemes suffer of the usual order barrier for A-stable methods. In particular, in [6] it was proved that the order of an A-stable convolution quadrature cannot exceed 2. Clearly, this result represents an extension of the famous second Dahlquist barrier for linear multistep methods (LMMs) for ordinary differential equations. This latter barrier can be overcomed if LMMs are used as Boundary Value Methods (BVMs) that is if the discrete problem generated by a k-step LMM is completed by imposing k_1 and $k_2 = k - k_1$ boundary conditions, [1]. In this paper, we shall investigate if the BVM approach is successfull in overcoming the barrier established in [6] for convolution quadrature methods. In particular, we shall consider the application of a generalized version of implicit Adams product quadrature rule that we call *Fractional Generalized Adams methods* (FGAMs).

FRACTIONAL GENERALIZED ADAMS METHODS

For each $t \in [0,T]$, let

$$J[\phi](t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-u)^{\alpha-1} \phi(u) du, \qquad \phi(u) = f(u, y(u)). \tag{5}$$

In addition, for the assigned uniform partition in (3), let

$$J^{(m)}[\phi](t) = \frac{1}{\Gamma(\alpha)} \int_{t_{m-1}}^{t_m} (t-u)^{\alpha-1} \phi(u) du, \qquad m = 1, \ldots, N.$$

It is evident that

$$J[\phi](t_n) = \sum_{m=1}^{n} J^{(m)}[\phi](t_n), \qquad n = 1, \ldots, N. \tag{6}$$

In order to compute an approximation of $J^{(m)}[\phi](t_n)$, we consider the application of a generalized version of the implicit k-step Adams product quadrature rule given by

$$J^{(m)}[\phi](t_n) \approx h^{\alpha} \sum_{j=0}^{k} \beta_{j,r} \phi_{m+k_2-j} =: \Omega_n^{(m)}[\phi], \qquad n \geq m \geq k_1, \quad r = n-m+1, \qquad k_1 + k_2 = k, \tag{7}$$

where $\phi_s = \phi(t_s)$ for each $s \geq 0$. The coefficients $\beta_{j,r}$ are uniquely determined by imposing the method to be consistent of order $p = k+1$, namely if $\phi \in C^p(I)$ then

$$J^{(m)}[\phi](t_n) - \Omega_n^{(m)}[\phi] = \tau_n^{(m)} \leq K h^{p+\alpha} \tag{8}$$

being K a constant independent of h. It is possible to prove that the coefficients $\beta_{j,r}$'s behave asymptotically as $\beta_{j,r} \sim r^{\alpha-1}$. Moreover, the resulting local truncation error in (8) is given by

$$\tau_n^{(m)} = \theta^{(r)} h^{p+\alpha} D^p \phi(\xi_{m,n}), \qquad \xi_{m,n} \in [t_{m-1}, t_m], \tag{9}$$

where the principal error coefficients $\theta^{(r)}$ verifies $\theta^{(r)} \sim r^{\alpha-1}$. It is to be noted that for $\alpha = 1$ and

$$k_1 = \lceil k/2 \rceil = \lfloor p/2 \rfloor, \qquad k_2 = k - k_1 = \lfloor (p-1)/2 \rfloor \tag{10}$$

the resulting methods are the Generalized Adams Methods (GAMs) for ODEs introduced in [1]. After some computations, one verifies that

$$\sum_{m=k_1}^{n} J^{(m)}[\phi](t_n) \approx \sum_{m=k_1}^{n} \Omega_n^{(m)} = h^{\alpha} \sum_{j=0}^{k-1} \bar{w}_{n,j} \phi_j + h^{\alpha} \sum_{j=0}^{n+k_2} \omega_{n-j} \phi_j$$

where, for each $j = 0, 1, \ldots, k-1$, and $s \geq -k_2$

$$\bar{w}_{n,j} = - \sum_{i=j-k_2}^{k_1-1} \beta_{i+k_2-j, n-i+1}, \qquad \omega_s = \sum_{i=0}^{\min(k, s+k_2)} \beta_{i, s+k_2+1-i}. \tag{11}$$

The fractional convolution quadrature we have considered for approximating (6) is given by

$$J[\phi](t_n) \approx J_n[\phi] := h^\alpha \sum_{j=0}^{M} w_{n,j}\phi_j + h^\alpha \sum_{j=0}^{n+k_2} \omega_{n-j}\phi_j =: h^\alpha \sum_{j=0}^{M} w_{n,j}\phi_j + \Omega_n[\phi] \tag{12}$$

where M depends on k and α as described later on. From (11) and the previous consideration on the asymptotic behaviour of the coefficients $\beta_{j,r}$'s, one immediately deduces that the convolution part $\Omega_n[\phi]$ is *stable* [6] (with respect to $J[\phi]$) since its weights verify

$$\omega_n = O(n^{\alpha-1}), \qquad n>0, \quad \text{and} \quad \omega_n = O(1), \quad -k_2 \le n \le 0.$$

Moreover, it is possible to prove that it is *convergent of order p* since, for all $\phi(t) = t^{\lambda-1}$, with $\lambda > 0$,

$$\Delta_n[\phi] := J[\phi](t_n) - \Omega_n[\phi] = O(h^\lambda) + O(h^p), \qquad t_n = nh \in [a,T], \quad a>0 \quad \text{fixed}.$$

The overall truncation (or quadrature) error associated to (12) is given by

$$E_n[\phi] = J[\phi](t_n) - J_n[\phi] = \Delta_n[\phi] - h^\alpha \sum_{j=0}^{M} w_{n,j}\phi_j.$$

It is known that if $y(t)$ is the exact solution of (2) with $f(t,y)$ smooth enough, then $\phi(t) = f(t,y(t))$ is generated by functions of the form $\phi_{\mu,\ell}(t) = t^{\mu+\ell\alpha}$ where μ and ℓ are nonnegative integers. This means that $\phi(t)$ contains nonsmooth components in proximity of the origin. It follows that the starting quadrature must be chosen appropriately, in order to get a convolution quadrature for which $E_n[\phi] = O(h^p)$ uniformly for all $nh \ge a > 0$. This objective is gained by imposing

$$E_n[\phi_{\mu,\ell}] = 0, \qquad \text{for all } (\mu,\ell) \in M_p(\alpha) \tag{13}$$

where $M_p(\alpha) = \{(\mu,l) : l \le l_p(\alpha), \mu \le \mu_p(\alpha,l)\}$ with $\mu_p(\alpha,l) = p-1-l\alpha$ and $l_p(\alpha) = (p-1)/\alpha$ if α is irrational or $l_p(\alpha) = \min(q-1,(p-1)/\alpha)$ if $\alpha = m/q$ with m and q coprime. If we set $M = \#M_p(\alpha) - 1$, then the conditions in (13) uniquely determine the starting weights $w_{n,j}$, $j = 0,1,\dots,M$, for each $n \ge M+1$. It is possible to prove that $w_{n,j}$ are independent of h and $w_{n,j} = O(n^{\alpha-1})$. Moreover, for any function $\phi(t) = \sum_{l=0}^{M} \tilde{\phi}_l(t) t^{l\alpha}$, with $\tilde{\phi}_l \in C^p(I)$, $E_n[\phi] = O(h^p)$ uniformly for any $nh \in [a,T]$ with $a > 0$ fixed. ANDREBBE MESSO IL COMPORTAMENTO DI E_n SENZA IL VINCOLO $nh > a > 0$?? These results are in perfect agreement with those obtained for fractional linear multistep method in [6].

CONVERGENCE ANALYSIS

We consider, for simplicity, the case where the FDE is scalar. If we denote with $e_n = y(t_n) - y_n$ the global error at $t = t_n$, and with L the Lipschitz constant of $f(t,y)$ then it is not difficult to verify that, see (4),

$$|e_n| \le h^\alpha L \left(\sum_{j=0}^{\min(n+k2,N-k_2)} |\omega_{n-j}||e_j| \right) + g_n + |E_n|, \qquad n = M+1,\dots,N-k_2, \tag{14}$$

being E_n the nth truncation error of the convolution quadrature whose behaviour, with respect to h, has been studied in the previous section, and $g_n = h^\alpha L \left(\sum_{j=0}^{M} |w_{n,j} - \omega_{n-j}||e_j| \right) + h^\alpha L \left(\sum_{j=N-k_2+1}^{n+k_2} |\omega_{n-j}||e_j| \right)$. If we assume to know an approximation of the first M and the last k_2 values of the numerical solution with accuracy $O(h^{p-\alpha})$ then $g_n = O(h^p)$ for each n. The system of inequalities in (14) can be rewritten in matrix form as

$$Z\mathbf{e} \le \mathbf{g} + E,$$

where $\mathbf{e} = \left(|e_{M+1}|,\dots,|e_{N-k_2}|\right)^T$, $\mathbf{g} = \left(g_{M+1},\dots,g_{N-k_2}\right)^T$, $E = \left(|E_{M+1}|,\dots,|E_{N-k_2}|\right)^T$, and $Z = (z_{i,j})$ is a Toeplitz matrix with $z_{i,j} = 0$ for each $j - i > k_2$. It is possible to prove that if h is "sufficiently" small then $Z^{-1} \ge O$ and $\|Z^{-1}\|_\infty$ is bounded. Clearly, this implies that

$$\|\mathbf{e}\|_\infty \le K\left(\|\mathbf{g}\|_\infty + \|E\|_\infty\right),$$

being K a suitable constant independent of h.

LINEAR STABILITY ANALYSIS

Let us consider the application of the method to the scalar test equation

$$D_0^\alpha y(t) = \lambda y(t).$$

It is known that for $\lambda \in \mathscr{S}_\alpha = \left\{\mu \in \mathbb{C} : |\arg(\mu - \pi)| < \left(1 - \frac{\alpha}{2}\right)\pi\right\}$ the exact solution satisfies $y(t) \to 0$ as $t \to 0$. When applied to the test equation, the discrete problem generated by a k-step FGAM used with k_2 final conditions reads

$$\begin{aligned} y_n &= g_n + q\sum_{j=0}^{n+k_2} \omega_{n-j} y_j, \qquad g_n = y_0 + q\sum_{j=0}^{M} w_{n,j} y_j, \qquad n = M+1, \ldots, N-k_2, \qquad q = h^\alpha \lambda. \\ & y_0, \ldots, y_M, \qquad y_{N-k_2+1}, \ldots, y_N \quad \text{fixed} \end{aligned}$$

It is evident that $y_n \equiv y_{n,N}(q)$ for each $n = M+1, \ldots, N-k_2$. The *region of absolute stability* of the method, say $\mathscr{D}_\alpha$, is the set of all $q \in \mathbb{C}$ for which there exists a sequence $\{v_n(q)\}_{n\geq 0}$ independent of N such that $v_n(q) \to 0$ as $n \to 0$, and $|y_{n,N}(q)| \leq |v_n(q)|$ whenever n and $N-n$ are sufficiently large. Clearly, the exact and the numerical solutions have the same qualitative behaviour for each $q \in \mathscr{S}_\alpha \cap \mathscr{D}_\alpha$. and the method is *A-stable* if $\mathscr{S}_\alpha \subseteq \mathscr{D}_\alpha$. If we denote with $\omega(\zeta)$ the generating power series of the convolution weights $\{\omega_n\}_{n\geq -k_2}$, i.e. $\omega(\zeta) = \sum_{j=0}^{\infty} \omega_{j-k_2} \zeta^j$, then the stability region is $\mathscr{D}_\alpha = \mathbb{C} \setminus \left\{\zeta^{k_2}/\omega(\zeta) : |\zeta| \leq 1\right\}$. In Figure 1, we have reported the boundary loci for the FGAMs of orders $p = 3$ and 5 used with $k_2 = \lfloor (p-1)/2 \rfloor$, see (10), final conditions for three values of α. As one can see, the methods are always *A*-stable.

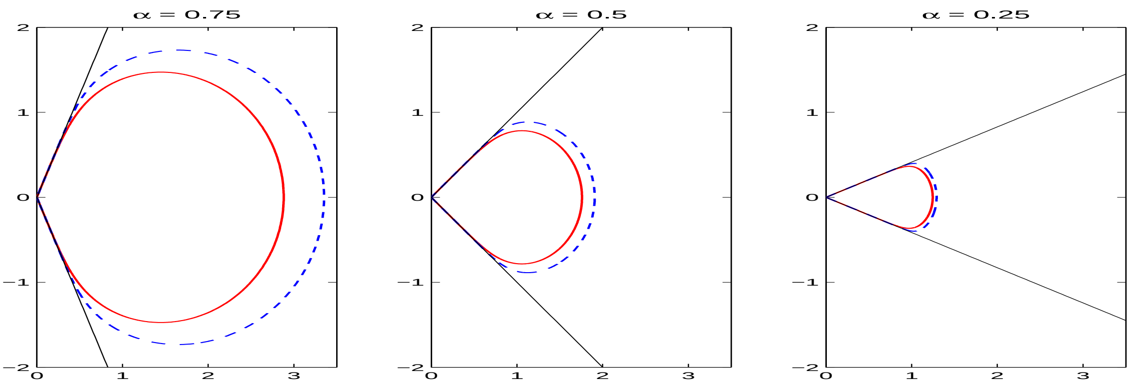

FIGURE 1. Boundary loci for the FGAMs of order $p = 3$ (solid line) and $p = 5$ (dashed line).

REFERENCES

1. L. Brugnano and D. Trigiante, Solving ODEs by Linear Multistep Initial and Boundary Value Methods, Amsterdam, Gordon & Breach, 1998.
2. H. Brunner, P.J. van der Houwen, The numerical solution of Volterra equations, CWI Monographs 3, North-Holland, Amsterdam, 1986.
3. M. Caputo,Linear models of dissipation whose Q is almost frequency independent, II. Geophys. J. Royal Astronom. Soc. 13 (1967) 529-539.
4. K. Diethelm, N.J. Ford, Analysis of fractional differential equations, J. Math. Anal. Appl. 265 (2002) 229-248.
5. C. Lubich, Fractional linear multistep methods for Abel-Volterra integral equations of the second kind, Math. Comp. 45 (1985) 463-469.
6. C. Lubich, Discretized fractional calculus, SIAM J. Math. Anal. 17 (1986) 704-719.
7. C. Lubich, A stability analysis of convolution quadrature for Abel-Volterra integral equations, IMA J. Numer. Anal. 6 (1986) 87-101.
8. I. Podlubny, Fractional Differential Equations, Academic Press, San Diego, 1999.