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Fractional multistep methods for weakly singular Volterra integral equations of the first kind with perturbed data

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Summary In this paper we consider the regularizing properties of fractional multistep methods for the stable solution of linear weakly singular Volterra integral equations of the first kind with perturbed right-hand sides.

1 Introduction

In this paper we consider linear weakly singular Volterra integral equations which are of the following form,

$$(Au)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-y)^{-(1-\alpha)} k(x,y) u(y) dy = f(x) \quad \text{for } 0 \leq x \leq L, \quad (1.1)$$

with $0 < \alpha < 1$ and some real number $L > 0$, and with a sufficiently smooth kernel function $k : [0, L] \times [0, L] \rightarrow \mathbb{R}$, and Γ denotes Euler's gamma function. For applications see e.g. Durbin [5] and Lerche/Zeitler [13], where crossing probabilities for Brownian motions and the inversion of the two-dimensional Radon transform are considered, respectively. In the sequel we will suppose that the kernel function does not vanish on the diagonal $0 \leq x = y \leq L$, and without loss of generality we then may assume that

$$k(x, x) = 1 \quad \text{for } 0 \leq x \leq L \quad (1.2)$$

holds. Moreover, the function $f : [0, L] \rightarrow \mathbb{R}$ is supposed to be known approximately, and a function $u : [0, L] \rightarrow \mathbb{R}$ satisfying equation (1.1) has to be determined.

There exists many classes of methods for the approximate solution of equation (1.1) if the right-hand side f is exactly given, see e.g., Brunner/van der Houwen [2] and Hackbusch [8]. One of these classes are fractional multistep methods which are introduced by C. Lubich ([14], [15]). In the present paper we review these methods (cf. Sections 2 and 3) and then consider their regularizing properties when the right-hand side in equation (1.1) is only approximately given (cf. Section 4). Finally fractional BDF methods are considered in more detail and numerical illustrations are presented (cf. Section 5).

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2 Review of a class of convolution quadrature methods and the basic notations

In this section we recall (with slight modifications occasionally) the basic notations and results from the paper [14].

2.1 Quadrature methods of convolution form

As a first step we consider in (1.1) the special situation $k \equiv 1$, with the corresponding integral operator being the classical Abel integral operator

$$(\mathcal{V}_\alpha u)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-y)^{-(1-\alpha)} u(y) dy \quad \text{for } 0 \leq x \leq L, \quad (2.1)$$

where $u : [0, L] \rightarrow \mathbb{R}$ is supposed to be a continuous function. For the numerical approximation of the integral $(\mathcal{V}_\alpha u)(x)$ with $0 \leq x \leq L$ we consider convolution quadrature methods of the form

$$(\Omega_h u)(x) = h^\alpha \sum_{j=0}^n \omega_{n-j} u(jh) \quad \text{for } h = x/n, \quad n = 1, 2, \dots \quad (2.2)$$

Here $\omega_0, \omega_1, \dots$ denotes an infinite sequence of real coefficients which is assumed to be independent of the considered point x and the stepsize h . More conditions on these weights as well as examples will be considered later in this subsection.

The error of the convolution quadrature method (2.2) at a point $0 \leq x \leq L$ is then given by

$$(E_h u)(x) = (\Omega_h u)(x) - (\mathcal{V}_\alpha u)(x) \quad \text{for } h = x/n, \quad n = 1, 2, \dots \quad (2.3)$$

The convergence order of a quadrature method (2.2) is determined by the error of the method with respect to monomials, see the following definition. As a preparation we note that the considered quadrature method of course may be applied to functions u which are defined on other intervals than $[0, L]$. In addition, the approximation $(\Omega_h u)(x)$ is independent of the right-hand endpoint L so that it is not necessary to refer to the particular choice of L , cf. Definition 1 below.

Definition 1 *The convolution quadrature method (2.2) for the numerical integration of (2.1) is called convergent of $p \geq 1$, if*

$$(E_h y^q)(1) = \mathcal{O}(h^{q+1}) \quad \text{as } h = 1/n \rightarrow 0 \quad (q = 0, 1, \dots, p-1). \quad (2.4)$$

Note that in (2.4) the error is considered only at the point $x = 1$. For a given sufficiently smooth function $u : [0, L] \rightarrow \mathbb{R}$ we next consider the error $(E_h u)(x)$ of the convolution quadrature method (2.2). This error can be written as follows,

$$(E_h u)(x) = \sum_{r=0}^{p-1} \frac{u^{(r)}(0)}{r!} (E_h y^r)(x) + (E_h R_p)(x) \quad \text{for } h = x/n, \quad (2.5)$$

for $n = 1, 2, \dots$, with the remainder $R_p(y) = \frac{1}{(p-1)!} \int_0^y (y-z)^{p-1} u^{(p)}(z) dz$. For a convolution quadrature method (2.2) of convergence order p , subsequently for each point $x = nh$ the weights for the starting values $u(jh)$ for $j = 0, 1, \dots, p-1$ will be modified to eliminate the errors $(E_h y^r)(x)$ for $r = 0, 1, \dots, p-1$, cf. Section 2.3 for more details. It then basically remains to consider the quadrature error of the remainder, which will be done first (cf. Section 2.2).

We conclude this subsection with some preparatory considerations. First, it turns out to be useful to extend the definition of the convolution quadrature method (2.2) to arbitrary step sizes h and points x as follows,

$$(\Omega_h u)(x) = h^\alpha \sum_{j=0}^{\lfloor x/h \rfloor} \omega_j u(x - jh) \quad \text{for } h > 0, \quad 0 \leq x \leq L, \quad (2.6)$$

where $\lfloor z \rfloor$ denotes the largest integer $\leq z$. The error $(E_h u)(x)$ considered in (2.3) then can easily be extended to arbitrary step sizes h by using the extended definition (2.6) of the considered quadrature method. For this extended definition of the considered quadrature method there holds

$$(E_h(u * v))(x) = ((E_h u) * v)(x) \quad \text{for } h > 0, \quad 0 \leq x \leq L \quad (2.7)$$

for continuous functions $u, v : [0, L] \rightarrow \mathbb{R}$. We recall that the convolution $\varphi * \psi : [0, L] \rightarrow \mathbb{R}$ of two arbitrary continuous functions $\varphi, \psi : [0, L] \rightarrow \mathbb{R}$ is given by $(\varphi * \psi)(x) = \int_0^x \varphi(x-y)\psi(y) dy$ for $0 \leq x \leq L$. Additionally for integers $q = 0, 1, \dots$ we have

$$(E_h y^q)(x) = x^{\alpha+q} (E_{h/x} y^q)(1) \quad \text{for } h > 0, \quad x > 0. \quad (2.8)$$

Both representations (2.7) and (2.8) follow from similar properties of the Abel integral operator and the quadrature method, respectively.

We need some properties of the weights $\omega_0, \omega_1, \dots$ considered in the convolution quadrature method (2.2), and for this purpose these weights are considered as the coefficients of a power series,

$$\omega(\xi) = \sum_{n=0}^{\infty} \omega_n \xi^n, \quad (2.9)$$

which is called the generating function of the quadrature method (2.2). We suppose that this power series converges for $|\xi| < 1$, and in addition in this paper we restrict the considerations to those generating functions $\omega(\xi)$ which can be represented as follows,

$$\omega(\xi) = (1 - \xi)^{-\alpha} \tilde{\omega}(\xi), \quad \tilde{\omega}(\xi) \text{ holomorphic on } \mathbf{B}_{1+\varepsilon} = \{\xi \in \mathbb{C} : |\xi| < 1 + \varepsilon\}, \quad (2.10)$$

$$\tilde{\omega}(\xi) \neq 0 \quad \text{for } \xi \in \mathbf{B}_{1+\varepsilon}, \quad (2.11)$$

with some real number $\varepsilon > 0$. The representation (2.10)–(2.11) has implications on the decay of the coefficients ω_n ,

$$\omega_n = a n^{-(1-\alpha)} + \mathcal{O}(n^{-(2-\alpha)}) \quad \text{as } n \rightarrow \infty \quad (2.12)$$

with some real constant $a \neq 0$. In fact, (2.12) is a stability property. Examples of generating functions satisfying (2.10)–(2.11) are given in Section 5.

2.2 Application of the considered quadrature method to the Taylor expansion remainder: an error analysis

We next present an error representation of the convolution quadrature method (2.2) applied to the Taylor expansion remainder considered in (2.5). This representation differs from the error expansion considered in [15] and requires in the subsequent proofs slightly less smoothness of the involved functions. For an integer $r \geq 1$, in the following $C^r[0, L]$ denotes the set of r -times continuously differentiable functions $f : [0, L] \rightarrow \mathbb{R}$.

2.3 Starting weights

In the sequel the convolution quadrature method $(\Omega_h u)(x)$ given by (2.2) is considered at uniformly distributed grid points $x = nh$ for $n = 1, 2, \dots, N$, where the integer N and the step size h are related as follows,

$$h = L/N.$$

In addition we suppose that the convolution quadrature method $(\Omega_h u)(x)$ has convergence order p and consider then the modification

$$(\tilde{\Omega}_h u)(x) := \overbrace{h^\alpha \sum_{j=0}^n \omega_{n-j} u(jh)}^{= (\Omega_h u)(x)} + h^\alpha \sum_{j=0}^{p-1} w_{n,j} u(jh) \quad \text{for } x = nh \quad (2.15)$$

as approximations to the fractional integral $(\mathcal{V}_\alpha u)(x)$ for $x = nh$ with $n = 1, 2, \dots, N$, respectively. Here, $w_{n,j}$ for $j = 0, 1, \dots, p-1$ are certain correction weights for the starting values to be specified. Due to the form of the second sum in (2.15) it is necessary to impose the technical condition $h(p-1) \leq L$.

In the modified quadrature method (2.15), for each $n = 1, 2, \dots, N$ a reasonable approach is to choose starting weights such that (2.15) is exact at $x = nh$ for all polynomials of degree $\leq p-1$, i.e.,

$$(\tilde{\Omega}_h y^q)(x) = (\mathcal{V}_\alpha y^q)(x) \quad \text{for } q = 0, 1, \dots, p-1. \quad (2.16)$$

This means

$$\sum_{j=0}^{p-1} w_{n,j} j^q = \frac{\Gamma(q+1)}{\Gamma(\alpha+q+1)} n^{\alpha+q} - \sum_{j=0}^n \omega_{n-j} j^q \quad \text{for } q = 0, 1, \dots, p-1, \quad (2.17)$$

which in fact is a linear system of p equations for the unknowns $w_{n,j}$, $j = 0, 1, \dots, p-1$ with a Vandermonde matrix which does not depend on n . Since the right-hand side of the identity in (2.17) is $\mathcal{O}(n^{-(1-\alpha)})$, there holds the estimate

$$w_{n,j} = \mathcal{O}(n^{-(1-\alpha)}) \quad \text{as } n \rightarrow \infty \quad \text{for } j = 0, 1, \dots, p-1. \quad (2.18)$$

Note that the considered approach for determining the starting weights cannot be applied in the case $x = 0$. In that case one obtains $(\tilde{\Omega}_h y^q)(0) = 0$ for $q = 0, 1, \dots, p-1$ which cannot be used in the subsequent considerations on the numerical solution of integral equations of the first kind.

We now consider the error of the modified quadrature method,

$$(\tilde{E}_h u)(x) = (\tilde{\Omega}_h u)(x) - (\mathcal{V}_\alpha u)(x) \quad \text{for } h = x/n, \quad n = 1, 2, \dots.$$

For fixed step size h this error can be written as

$$(\tilde{E}_h u)(x) = (E_h R_p)(x) + h^\alpha \sum_{j=0}^{p-1} w_{n,j} R_p(jh). \quad (2.19)$$

With the same assumptions as in Proposition 1, the first term on the right-hand side of (2.19) can be written in the form $c_p h^{p+\alpha} \sum_{j=0}^n \omega_{n-j} u^{(p)}(jh) + \mathcal{O}(h^{p+\alpha})$. In addition, the sum in (2.19)

is of the form $\mathcal{O}(h^{p+1})$ which follows from (2.18). As an immediate result we obtain the following representation of the error of the modified quadrature method:

$$(\tilde{E}_h u)(x) = c_p h^{p+\alpha} \sum_{j=0}^n \omega_{n-j} u^{(p)}(jh) + \mathcal{O}(h^{p+\alpha}) \quad \text{for } x = nh, \\ n = 0, 1, \dots, N, \quad (2.20)$$

for $h \rightarrow 0$ uniformly with respect to x , with some real constant c_p .

3 Numerical solution of weakly Volterra integral equations of the first kind by the modified quadrature method

3.1 Introductory remarks and the basic algorithm

In this section we recall the basic result of the paper [15]. For this purpose we again consider the weakly singular Volterra integral equation of the first kind (1.1) and suppose that it has a unique solution $u : [0, L] \rightarrow \mathbb{R}$ (sufficient conditions are given at the end of Section 4). Additionally we suppose that the values of the right-hand side of equation (1.1) are exactly given at uniformly distributed grid points

$$x_n = nh \quad \text{for } n = 1, 2, \dots, N, \quad (3.1)$$

respectively. In the sequel we consider a convolution quadrature method of the form (2.2) which has convergence order p . In addition modified starting weights as in (2.15) are used to determine approximations $u_n \approx u(x_n)$ for $n = 1, 2, \dots, N$. This means that for a given starting value $u_0 \approx u(0)$, approximations u_1, u_2, \dots, u_N have to be determined such that the identities

$$h^\alpha \sum_{j=0}^n \omega_{n-j} k(x_n, x_j) u_j + h^\alpha \sum_{j=0}^{p-1} w_{n,j} k(x_n, x_j) u_j = f(x_n) \quad (3.2)$$

are satisfied for $n = 1, 2, \dots, N$. Note that the assumption $k \equiv 1$ is now omitted, and the general situation for the kernel k is considered in the sequel. The procedure for determining these approximations is as follows:

- (a) First determine a starting value $u_0 \approx u(0)$. One of the reasonable algorithms is considered at the end of Section 4.
- (b) Then solve (3.2) for $n = 1, 2, \dots, p-1$. This leads to a linear system of $p-1$ equations for the $p-1$ unknowns u_1, u_2, \dots, u_{p-1} .
- (c) The identities (3.2) then are used successively for $n = p, p+1, \dots, N$ to determine the approximations u_p, u_{p+1}, \dots, u_N , respectively.

We next present the approximation properties of the scheme (3.2). As a preparation we formulate the basic assumptions.

- Assumption 1** (a) *The convolution quadrature method (2.2) is convergent of order $p \geq 1$,*
 (b) *the corresponding generating function $\omega(\xi)$ considered in (2.9) can be represented as in (2.10)–(2.11),*
 (c) *the starting weights are determined according to the conditions in (2.16),*
 (d) *the kernel function k in the integral operator (1.1) has continuous partial derivatives up to the order $p+1$ on $[0, L] \times [0, L]$, and the solution u of the integral equation (1.1) is $(p+1)$ -times continuously differentiable on the interval $[0, L]$,*

(e) and $k(x, x) = 1$ holds for each $0 \leq x \leq L$.

At the end of Section 4, conditions on the right-hand side of the considered weakly singular Volterra integral equation of the first kind are given which guarantee the existence of a solution u satisfying (d) in Assumption 1.

As another preparation we present a useful result on the quadrature error for general kernels k . For this we introduce notations for the error of the scheme (3.2),

$$e_n := u(x_n) - u_n \quad \text{for } n = 0, 1, \dots, N. \quad (3.3)$$

If the conditions in Assumption 1 are satisfied, then there holds

$$\begin{aligned} & h^\alpha \sum_{j=0}^n \omega_{n-j} k(x_n, x_j) e_j + h^\alpha \sum_{j=0}^{p-1} w_{n,j} k(x_n, x_j) e_j \\ &= c_p h^{p+\alpha} \sum_{j=0}^n \omega_{n-j} \varphi(x_j) + \mathcal{O}(h^{p+\alpha}) \quad \text{for } n = 1, 2, \dots, N \end{aligned} \quad (3.4)$$

uniformly with respect to n , with the function $\varphi(x) = \frac{d^p}{dy^p} \{k(x, y)u(y)\}_{|y=x}$ for $0 \leq x \leq L$. For each n the representation (3.4) follows from the representation (2.20), with the function u replaced by the function $y \mapsto k(x_n, y)u(y)$ considered on the interval $[0, x_n]$ there.

3.2 Uniqueness, existence and approximation properties of the starting values

We now consider uniqueness, existence and approximation properties of the starting values u_1, u_2, \dots, u_{p-1} . As a first step we consider in more detail the linear system of equations

$$h^\alpha \sum_{j=0}^{p-1} \underbrace{(\omega_{n-j} + w_{n,j})}_{=: \bar{\omega}_{n,j}} k(x_n, x_j) u_j = f(x_n) \quad \text{for } n = 1, 2, \dots, p-1, \quad (3.5)$$

with the notation $\omega_n = 0$ for $n < 0$. The linear system of equations (3.5) can be written in the form

$$\begin{aligned} & \overbrace{\left[\begin{array}{cccc} \bar{\omega}_{1,1} k_{1,1} & \bar{\omega}_{1,2} k_{1,2} & \cdots & \bar{\omega}_{1,p-1} k_{1,p-1} \\ \bar{\omega}_{2,1} k_{2,1} & \bar{\omega}_{2,2} k_{2,2} & \cdots & \bar{\omega}_{2,p-1} k_{2,p-1} \\ \vdots & \vdots & & \vdots \\ \bar{\omega}_{p-1,1} k_{p-1,1} & \bar{\omega}_{p-1,2} k_{p-1,2} & \cdots & \bar{\omega}_{p-1,p-1} k_{p-1,p-1} \end{array} \right]} =: S \\ & h^\alpha \left(\begin{array}{c} u_1 \\ u_2 \\ \vdots \\ u_{p-1} \end{array} \right) = \left(\begin{array}{c} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{p-1}) \end{array} \right) - h^\alpha \left(\begin{array}{c} \bar{\omega}_{1,0} k_{0,0} \\ \bar{\omega}_{2,0} k_{1,0} \\ \vdots \\ \bar{\omega}_{p-1,0} k_{p-1,0} \end{array} \right) u_0 \end{aligned} \quad (3.6)$$

with the notation

$$k_{n,j} = k(x_n, x_j) \quad \text{for } 0 \leq j, n \leq p-1.$$

It turns out that the matrix $S = S(h) \in \mathbb{R}^{(p-1) \times (p-1)}$ in (3.6) is non-singular for sufficiently small values h , and $\|S^{-1}\|_\infty = \mathcal{O}(h^{-\alpha})$ holds for $h \rightarrow 0$ where $\|\cdot\|_\infty$ denotes the matrix norm induced by the maximum norm for vectors. This estimate for the matrix S^{-1} is obtained by considering first the case $k \equiv 1$ and applying the representation (2.17), and the general case is then obtained by using a perturbation argument.

We now present the approximation properties of the considered starting values u_1, u_2, \dots, u_{p-1} .

Proposition 2 *Let Assumption 1 be satisfied, let u_0 be a starting value with $u_0 - u(x_0) = \mathcal{O}(h^p)$ as $h \rightarrow 0$, and let the other starting values u_1, u_2, \dots, u_{p-1} be determined by (3.2) for $n = 1, 2, \dots, p-1$. Then there holds*

$$\max_{n=1,2,\dots,p-1} |u_n - u(x_n)| = \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0. \quad (3.7)$$

Proof We repeat from [15] the basic steps of the proof since some of these steps are also needed in the proof of the main result in the present paper (cf. Section 4). The error representation (3.4) and the assumptions on the approximation properties of the starting value u_0 yield

$$h^\alpha \sum_{j=1}^{p-1} \bar{\omega}_{n,j} k(x_n, x_j) e_j = \mathcal{O}(h^{p+\alpha}) \quad \text{for } n = 1, 2, \dots, p-1. \quad (3.8)$$

A matrix-vector formulation of (3.8) gives

$$\|SE_h\|_\infty = \mathcal{O}(h^{p+\alpha}) \quad \text{as } h \rightarrow 0, \quad \text{with } E_h := (e_1, e_2, \dots, e_{p-1})^\top$$

with the matrix S from (3.6) which is non-singular for sufficiently small values h , with $\|S^{-1}\|_\infty = \mathcal{O}(h^{-\alpha})$ as $h \rightarrow 0$, see the statements above. Here and in the sequel, $\|\cdot\|_\infty$ denotes the maximum norm for vectors as well as the induced matrix norm, respectively. From this the estimate (3.7) follows. \square

3.3 The approximation properties of the values u_p, u_{p+1}, \dots, u_N

We now present the main result on the convergence order of the approximations obtained by the scheme (3.2). As a preparation consider the reciprocal

$$\frac{1}{\omega(\xi)} = \sum_{n=0}^{\infty} \omega_n^{(-1)} \xi^n$$

of the generating function $\omega(\xi) = \sum_{n=0}^{\infty} \omega_n \xi^n$. It is an immediate consequence of the representation (2.10)–(2.11) that the coefficients of the reciprocal function $1/\omega(\xi)$ satisfy

$$\omega_n^{(-1)} = \mathcal{O}(n^{-\alpha-1}) \quad \text{as } n \rightarrow \infty. \quad (3.9)$$

We now present a special version of the main result of the paper by Lubich [15]:

Theorem 2 *Let the conditions of Proposition 2 be satisfied. Then the approximations u_p, u_{p+1}, \dots, u_N (determined by (3.2) for $n = p, p+1, \dots, N$, respectively) can be estimated as follows,*

$$\max_{n=p, p+1, \dots, N} |u_n - u(x_n)| = \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0.$$

Proof Again some of the steps in this proof are needed also in Section 4, therefore we repeat from [15] the basic steps of the proof. Moving the second sum on the left-hand side of the error representation (3.4) to the right-hand side gives the following error representation,

$$h^\alpha \sum_{j=0}^n \omega_{n-j} k(x_n, x_j) e_j = c_p h^{p+\alpha} \sum_{j=0}^n \omega_{n-j} \varphi(x_j) + \mathcal{O}(h^{p+\alpha}) \quad \text{for } n = 0, 1, \dots, N \quad (3.10)$$

for $h \rightarrow 0$ uniformly with respect to n . We next consider a matrix-vector formulation of (3.10). As a preparation we consider the matrix $A_h^\alpha \in \mathbb{R}^{(N+1) \times (N+1)}$ with

$$A_h^\alpha = h^\alpha \begin{bmatrix} \omega_0 k_{0,0} & 0 & \cdots & \cdots & \cdots & 0 \\ \omega_1 k_{1,0} & \omega_0 k_{1,1} & 0 & & & 0 \\ \vdots & \omega_1 k_{2,1} & \omega_0 k_{2,2} & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & 0 \\ \omega_N k_{N,0} & \cdots & \cdots & \cdots & \omega_1 k_{N,N-1} & \omega_0 k_{N,N} \end{bmatrix}$$

with the notation

$$k_{n,j} = k(x_n, x_j) \quad \text{for } 0 \leq j \leq n \leq N.$$

Additionally we consider the matrix $B_h^\alpha \in \mathbb{R}^{(N+1) \times (N+1)}$ given by

$$B_h^\alpha = h^\alpha \begin{bmatrix} \omega_0 & 0 & \cdots & \cdots & \cdots & 0 \\ \omega_1 & \omega_0 & 0 & & & 0 \\ \omega_2 & \omega_1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ \omega_N & \cdots & \cdots & \omega_2 & \omega_1 & \omega_0 \end{bmatrix},$$

and the vectors

$$E_h = (e_0, e_1, \dots, e_N)^\top, \quad G = c_p h^p (\varphi(x_0), \varphi(x_1), \dots, \varphi(x_N))^\top.$$

Using all these notations, the linear system (3.10) becomes

$$A_h^\alpha E_h = B_h^\alpha G + F_h^\alpha, \quad \text{with some } F_h^\alpha \in \mathbb{R}^{N+1}, \quad \|F_h^\alpha\|_\infty = \mathcal{O}(h^{p+\alpha}) \quad \text{as } h \rightarrow 0. \quad (3.11)$$

For a further treatment of the identity (3.11) we now consider the inverse matrix of B_h^α , this is $D_h^\alpha \in \mathbb{R}^{(N+1) \times (N+1)}$ with

$$D_h^\alpha = h^{-\alpha} \begin{bmatrix} \omega_0^{(-1)} & 0 & \cdots & \cdots & \cdots & 0 \\ \omega_1^{(-1)} & \omega_0^{(-1)} & 0 & & & 0 \\ \omega_2^{(-1)} & \omega_1^{(-1)} & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ \omega_N^{(-1)} & \cdots & \cdots & \omega_2^{(-1)} & \omega_1^{(-1)} & \omega_0^{(-1)} \end{bmatrix}. \quad (3.12)$$

We now apply the matrix D_h^α to both sides of (3.11) and obtain

$$\|D_h^\alpha A_h^\alpha E_h\|_\infty = \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0, \quad (3.13)$$

where the estimates

$$\|D_h^\alpha\|_\infty = \mathcal{O}(h^{-\alpha}), \quad \|G\|_\infty = \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0 \quad (3.14)$$

have been used, and the first estimate in (3.14) follows from the decay (3.9) of the coefficients of the reciprocal of the generating function ω . It then turns out (cf. Eggermont [6] for more details) that the lower triangular matrix $D_h^\alpha A_h^\alpha$ can be written as follows

$$D_h^\alpha A_h^\alpha = I + hK_h \quad \text{with } K_h = (k_{h,\ell,j}) \in \mathbb{R}^{(N+1) \times (N+1)} \text{ strictly lower triangular,} \\ \max_{1 \leq j < \ell \leq N+1} |k_{h,\ell,j}| = \mathcal{O}(1) \quad \text{as } h \rightarrow 0.$$

This representation and the discrete version of Gronwall's inequality now yields

$$\|(D_h^\alpha A_h^\alpha)^{-1}\|_\infty = \mathcal{O}(1) \quad \text{as } h \rightarrow 0. \quad (3.15)$$

The statement of the theorem now follows from the estimates (3.13) and (3.15). \square

Remark 2 (a) For the product-trapezoidal rule, a similar approach as in the proof of Theorem 2 is considered in Eggermont [6].

(b) It follows from the proof of Theorem 2 that in the situation of Assumption 1 the scheme (3.2) can be applied for $n = p, p+1, \dots, N$ with starting values u_1, u_2, \dots, u_{p-1} that are obtained by other approaches. The only requirement is that estimate (3.7) is satisfied.

4 Perturbed data

We now start with the main purpose of the present paper, this is, the consideration of the regularizing properties of the scheme (3.2). Here we consider the situation that only perturbed data f_n^δ are available at the grid points x_n , respectively, with

$$|f_n^\delta - f(x_n)| \leq \delta \quad \text{for } n = 1, 2, \dots, N, \quad (4.1)$$

where $\delta > 0$ is a known noise level. In that situation the discrete equations (3.2) are modified as follows: For some given starting value $u_0^\delta \approx u(0)$ determine approximations $u_n^\delta \approx u(x_n)$ for $n = 1, 2, \dots, N$ such that the identities

$$h^\alpha \sum_{j=0}^n \omega_{n-j} k(x_n, x_j) u_j^\delta + h^\alpha \sum_{j=0}^{p-1} w_{n,j} k(x_n, x_j) u_j^\delta = f_n^\delta \quad (4.2)$$

are satisfied for $n = 1, 2, \dots, N$. The procedure for determining these approximations is similar to the procedure for exactly given right-hand sides, cf. Section 3.1.

We are now in a position to formulate the main results of this paper. As a preparation we consider the following assumptions:

- Assumption 3** (a) *The conditions in Assumption 1 are satisfied,*
 (b) *the conditions (4.1) on the noise are satisfied,*
 (c) *and u_0^δ is a starting value with $u_0^\delta - u(x_0) = \mathcal{O}(h^p + \delta/h^\alpha)$ as $(h, \delta) \rightarrow 0$.*

The following proposition provides an error estimate for the starting values.

Proposition 3 *Let the conditions of Assumption 3 be satisfied, and let starting values $u_1^\delta, u_2^\delta, \dots, u_{p-1}^\delta$ be given by (4.2) for $n = 1, 2, \dots, p-1$, respectively. Then there holds*

$$\max_{n=1,2,\dots,p-1} |u_n^\delta - u(x_n)| = \mathcal{O}\left(h^p + \frac{\delta}{h^\alpha}\right) \quad \text{as } (h, \delta) \rightarrow 0.$$

Proof Due to the results in [15] which are recalled in the present paper it is sufficient to estimate the differences between the perturbed and the unperturbed approximations,

$$\Delta_n^\delta := u_n^\delta - u_n \quad \text{for } n = 1, 2, \dots, p-1.$$

Here the approximations u_1, u_2, \dots, u_{p-1} satisfy the unperturbed discrete equations (3.2), and u_0 denotes an arbitrary starting value with $u_0 - u(x_0) = \mathcal{O}(h^p)$ as $h \rightarrow 0$. A comparison of the identities (4.2) and (3.2) gives

$$h^\alpha \sum_{j=1}^{p-1} \bar{w}_{n,j} k(x_n, x_j) \Delta_j^\delta = \mathcal{O}(h^{p+\alpha} + \delta) \quad \text{for } n = 1, 2, \dots, p-1, \quad (4.3)$$

where the weights $\bar{w}_{n,j}$ are introduced in (3.5). Note that the summation in (4.3) begins with $j = 1$. A matrix-vector formulation of (4.3) yields

$$\|SE_h^\delta\|_\infty = \mathcal{O}(h^{p+\alpha} + \delta) \quad \text{as } (h, \delta) \rightarrow 0, \quad \text{with } E_h^\delta = (\Delta_1^\delta, \Delta_2^\delta, \dots, \Delta_{p-1}^\delta)^\top,$$

with the matrix S from (3.6) which is non-singular for sufficiently small values h and satisfies $\|S^{-1}\|_\infty = \mathcal{O}(h^{-\alpha})$ as $h \rightarrow 0$, cf. Section 3. From this the statement of the proposition follows. \square

The following theorem provides an error estimate for the approximations $u_p^\delta, u_{p+1}^\delta, \dots, u_N^\delta$.

Theorem 4 *Let the conditions of Proposition 3 be satisfied. Then the error for the approximations given by (4.2) for $n = p, p+1, \dots, N$ can be estimated as follows:*

$$\max_{n=p,p+1,\dots,N} |u_n^\delta - u(x_n)| = \mathcal{O}\left(h^p + \frac{\delta}{h^\alpha}\right) \quad \text{as } (h, \delta) \rightarrow 0. \quad (4.4)$$

Proof Again it is sufficient to estimate the differences

$$\Delta_n^\delta := u_n^\delta - u_n \quad \text{for } n = 0, 1, \dots, N,$$

where the approximations u_1, u_2, \dots, u_N satisfy the unperturbed discrete equations (3.2) for $n = 1, 2, \dots, N$, and u_0 denotes an arbitrary starting value with $u_0 - u(x_0) = \mathcal{O}(h^p)$ as $h \rightarrow 0$. From that we obtain

$$h^\alpha \sum_{j=0}^n \omega_{n-j} k(x_n, x_j) \Delta_j^\delta = \mathcal{O}(h^{p+\alpha} + \delta) \quad \text{as } (h, \delta) \rightarrow 0 \quad \text{for } n = 0, 1, \dots, N \quad (4.5)$$

uniformly with respect to n . Here the assumptions on the approximation properties of the starting values and the boundedness of the starting weights are used, cf. (2.18). A matrix–vector formulation of (4.5) is as follows,

$$\|A_h^\alpha E_h^\delta\|_\infty = \mathcal{O}(h^{p+\alpha} + \delta) \quad \text{as } (h, \delta) \rightarrow 0, \quad \text{with } E_h^\delta = (\Delta_0^\delta, \Delta_1^\delta, \dots, \Delta_N^\delta)^\top, \quad (4.6)$$

with the same notations for the matrix $A_h^\alpha \in \mathbb{R}^{(N+1) \times (N+1)}$ as in the proof of Theorem 2 on the error of the considered scheme (3.2) with unperturbed data. From the estimate $\|(A_h^\alpha)^{-1}\|_\infty = \mathcal{O}(h^{-\alpha})$ as $h \rightarrow 0$ (cf. estimates (3.14) and (3.15) in the proof of Theorem 2) we finally obtain the estimate (4.4). \square

As an immediate consequence of Proposition 3 and Theorem 4 we obtain the following main result of this paper.

Corollary 1 *Let Assumption 3 be satisfied, and let $h = h(\delta)$ be step sizes with $h \sim \delta^{1/(p+\alpha)}$ as $\delta \rightarrow 0$. Then the error for the approximations (given by (4.2) for $n = 1, 2, \dots, N$, respectively) can be estimated as follows:*

$$\max_{n=0,1,\dots,N} |u_n^\delta - u(x_n)| = \mathcal{O}(\delta^{p/(p+\alpha)}) \quad \text{as } \delta \rightarrow 0.$$

Here $h \sim \delta^{1/(p+\alpha)}$ means that there exist real constants $c_2 \geq c_1 > 0$ such that $c_1 h \leq \delta^{1/(p+\alpha)} \leq c_2 h$ as $\delta \rightarrow 0$.

We conclude this section with some important remarks.

Remark 3 (a) It follows from the considered proofs that also starting values $u_1^\delta, u_2^\delta, \dots, u_{p-1}^\delta$ obtained by other schemes than (4.2) can be used. In the situation of Corollary 1 the only requirement is $u_n^\delta - u(x_n) = \mathcal{O}(\delta^{p/(p+\alpha)})$ as $\delta \rightarrow 0$ for $n = 1, 2, \dots, p-1$.

(b) The smoothness conditions on the solution u considered in Assumption 1 are satisfied (and additionally, the existence of the solution u can be guaranteed then), if the exact right–hand side f can be written in the form $f(x) = x^\alpha g(x)$ with a function $g \in C^{p+2}[0, L]$ and if in addition the kernel $k(x, y)$ has for $0 \leq y \leq x \leq L$ continuous partial derivatives up to the order $p+3$, cf. Atkinson [1] for the details.

(c) In the situation of part (b) of this remark there holds $\alpha g(0) = u(0)$ which follows by simple calculations. Thus, for general values of h a possible strategy for the determination of a starting value u_0^δ is to consider the interpolating polynomial P^δ of degree not larger than $p-1$ which satisfies $P^\delta(x_r) = f^\delta(x_r)/x_r^\alpha$ for $r = 1, 2, \dots, p$. The choice $u_0^\delta = \alpha P^\delta(0) = u(0) + \mathcal{O}(h^p + \delta/h^\alpha)$ then gives a starting value of sufficiently good accuracy.

(d) For other special regularization methods for the approximate solution of Volterra integral equations of the first kind with perturbed right-hand sides and with possibly weakly singular kernels, see e.g., Bughgeim [3], Gorenflo/Vessella [7], Lamm [12] and the references therein.

(e) The presented propositions and theorems can be extended to Volterra integral equations of the first kind without weak singularities, this is the case $\alpha = 1$ in the Volterra integral equation of the first kind (1.1). The corresponding proofs have to be modified at some places. For example, for the proof of estimate (3.15) we need (in the case $\alpha = 1$) that the coefficients of the generating function $\omega(\xi)$ and its reciprocal $1/\omega(\xi)$ can be written as follows,

$$\omega_n = a + \mathcal{O}(q^n), \quad \omega_n^{(-1)} = \mathcal{O}(q^n) \quad \text{as } n \rightarrow \infty \quad (4.7)$$

for some real number $0 < q < 1$ and $a \in \mathbb{R}$. The representations in (4.7) in fact follow from the representation (2.10)–(2.11). For the application of multistep methods to Volterra integral equations of the first kind without weak singularities and with exactly given right-hand sides see Wolkenfelt [17].

5 Examples of fractional multistep methods for weakly singular Volterra operators, and numerical experiments

5.1 Multistep methods for initial value problems

In this section we will consider special convolution quadrature methods of the form (2.2) for the numerical approximation of the Abel integral operator (2.1). As a preparation consider the simple initial value problem

$$f'(x) = u(x) \quad \text{for } 0 \leq x \leq L, \quad f(0) = 0, \quad (5.1)$$

where the function $u : [0, L] \rightarrow \mathbb{R}$ is given, and the function $f : [0, L] \rightarrow \mathbb{R}$ has to be determined. For the numerical solution of the initial value problem (5.1) we consider linear multistep methods which are of the following form,

$$\sum_{j=0}^m \alpha_j f_{n+j} = h \sum_{j=0}^m \beta_j u_{n+j} \quad \text{for } n = 0, 1, \dots, N - m, \quad (5.2)$$

with given real coefficients $\alpha_0, \alpha_1, \dots, \alpha_m$ and $\beta_0, \beta_1, \dots, \beta_m$, with $m \in \mathbb{N}$ and $\alpha_m \neq 0, \beta_m \neq 0$. For given starting values f_0, f_1, \dots, f_{m-1} , the identities (5.2) are used to determine successively for $n = m, m + 1, \dots, N$ approximations f_n to the numbers $f(x_n)$, respectively.

An important class of examples are BDF methods:

Example 1 For $m = 1, 2, \dots, 6$, the m -step BDF method for solving the initial value problem (5.1) is as follows, respectively:

$$\sum_{k=1}^m \frac{1}{k} \nabla^k f_{n+m} = h u_{n+m} \quad \text{for } n = 0, 1, \dots, N - m, \quad (5.3)$$

with the recursively defined backward differences. See e.g., Hairer / Nørsett / Wanner [10] or [16] for an introduction to BDF methods. For $m \leq 3$, the BDF methods are of the following form, respectively:

$$\begin{aligned} m = 1 : & & f_{n+1} - f_n &= h u_{n+1}; \\ m = 2 : & & \frac{1}{2}(3f_{n+2} - 4f_{n+1} + f_n) &= h u_{n+2}; \\ m = 3 : & & \frac{1}{6}(11f_{n+3} - 18f_{n+2} + 9f_{n+1} - 2f_n) &= h u_{n+3}. \end{aligned}$$

In particular, for $m = 1$ the implicit Euler scheme is obtained.

For an arbitrary multistep method, the numbers f_0, f_1, \dots, f_N can be written in an explicit form. For this purpose we consider the associated generating polynomials

$$\rho(\xi) = \sum_{j=0}^m \alpha_j \xi^j, \quad \sigma(\xi) = \sum_{j=0}^m \beta_j \xi^j \quad (5.4)$$

as well as the corresponding formal power series

$$\tau(\xi) = \frac{\sigma(1/\xi)}{\rho(1/\xi)} =: \sum_{s=0}^{\infty} \tau_s \xi^s. \quad (5.5)$$

It turns out that the approximations f_m, f_{m+1}, \dots, f_N given by (5.2) can be written in the explicit form $f_n = h \sum_{s=0}^n \tau_{n-s} u_s$ for $n = m, m+1, \dots, N$ provided that the starting values f_0, f_1, \dots, f_{m-1} are of similar form. As an example consider again the BDF methods. For each m there obviously holds $\sigma(\xi) = \xi^m$, and hence the corresponding formal power series is of the form

$$\tau(\xi) = [\xi^m \rho(1/\xi)]^{-1}. \quad (5.6)$$

Examining the representation (5.3) in more detail shows that $\xi^m \rho(1/\xi) = \sum_{k=1}^m (1-\xi)^k / k$ holds.

5.2 Fractional multistep methods

For a given multistep method (5.2) for solving the initial value problem (5.1) we now recall briefly the basic properties of the corresponding fractional multistep method. For this purpose we write the formal power series (5.5) as follows, $\tau(\xi) = \tau_0 (1 + q(\xi))$ with the coefficient $\tau_0 = \beta_m / \alpha_m$ which is assumed to be positive, $\tau_0 > 0$. The binomial formula then gives for $0 < \alpha < 1$

$$\tau(\xi)^\alpha = \tau_0^\alpha \sum_{n=0}^{\infty} \binom{\alpha}{n} q(\xi)^n =: \sum_{n=0}^{\infty} \omega_n \xi^n =: \omega(\xi). \quad (5.7)$$

The corresponding fractional multistep method (for the approximation of the Abel integral operator (2.1)) is by definition of the form $(\Omega_h u)(x) = h^\alpha \sum_{j=0}^n \omega_{n-j} u(jh)$, with coefficients $\omega_0, \omega_1, \dots$ as in (5.7). These coefficients can be computed in a stable way by Newton's method for formal power series, which now will be described briefly for BDF methods, cf. Hairer / Lubich / Schlichte [9]. In fact, for BDF methods the equation (5.7) can be written as

$$F(\omega(\xi)) := \omega(\xi)^{-1/\alpha} - \underbrace{\xi^m \rho(1/\xi)}_{=: \tilde{\rho}(\xi)} = 0. \quad (5.8)$$

In the case $\alpha = 1/M$ with $M \geq 2$ being some integer, the equation (5.8) easily can be solved by Newton's method for formal power series. This generates a sequence of formal power series $\omega^{[1]}(\xi), \omega^{[2]}(\xi), \dots$ which here takes the form

$$\omega^{[s+1]}(\xi) = (1 + \alpha) \omega^{[s]}(\xi) - \alpha \{ [\omega^{[s]}(\xi)]^{1+1/\alpha} \tilde{\rho}(\xi) \}_{2^{s+1}} \quad \text{for } s = 0, 1, \dots \quad (5.9)$$

Here, the notation $\{a(\xi)\}_r = \sum_{n=0}^r a_n \xi^n$ is used as a truncation of a given formal power series $a(\xi) = \sum_{n=0}^{\infty} a_n \xi^n$. In addition it can be shown (Henrici [11]) that the first 2^s coefficients of the formal power series $\omega^{[s]}(\xi)$ and the solution $\omega(\xi)$ of the equation (5.8) coincide if $\omega^{[0]}(\xi) \equiv 1/\tilde{\rho}(0)^\alpha$ is chosen in (5.9) as initial formal power series.

5.3 Convergence order and stability of fractional multistep methods

It is well-known (cf. [10]) that a multistep method (5.2) for solving the simple initial value problem (5.1) is consistent of order p if and only if

$$h\tau(e^{-h}) = 1 + \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0 \quad (5.10)$$

holds for the corresponding generating function (5.5). It is supposed here that the generating function $\tau(\xi)$ converges for $|\xi| < 1$. For the fractional power series $\omega(\xi) = \tau(\xi)^\alpha$ we then have

$$h^\alpha \omega(e^{-h}) = 1 + \mathcal{O}(h^p) \quad \text{as } h \rightarrow 0. \quad (5.11)$$

It is shown in Lubich [14] that a convolution quadrature method (2.2), with a generating function (2.9) that is representable as in (2.10)–(2.11) and satisfies (5.11), is convergent of order p .

We next consider the condition (2.10)–(2.11) on the representation for generating functions of fractional multistep methods, and we restrict here the considerations to fractional BDF methods with $m \leq 6$. It can be shown that the denominator in (5.6) always has $\xi = 1$ as a simple root, and all other roots belong to the exterior of the closed unit disc. The corresponding function $\tau(\xi)^\alpha$ can be written as

$$\tau(\xi)^\alpha = [\xi^m \rho(1/\xi)]^{-\alpha} = (1 - \xi)^{-\alpha} \tilde{\omega}(\xi).$$

From the binomial expansion it follows that the considered function $\tilde{\omega}(\xi)$ is holomorphic and has no roots in the disk $\mathbf{B}_{1+\varepsilon} = \{\xi \in \mathbb{C} : |\xi| < 1 + \varepsilon\}$, with some $\varepsilon > 0$. This finally gives the required representation (2.10)–(2.11) for the generating function $\tau(\xi)^\alpha$ of the considered fractional BDF method.

5.4 Numerical experiments

As an illustration of the main result considered in Corollary 1, we next present the results of some numerical experiments. We consider the following linear weakly singular Volterra integral equation of the first kind,

$$\int_0^x (x-y)^{-1/2} e^{-(x-y)} u(y) dy = e^{-x}(x^5 + x^7 + x^9) \quad \text{for } 0 \leq x \leq 1, \quad (5.12)$$

with exact solution

$$u(y) = e^{-y} \left(\frac{5!}{\Gamma(5.5)} y^{9/2} + \frac{6!}{\Gamma(6.5)} y^{11/2} + \frac{7!}{\Gamma(7.5)} y^{13/2} \right) \quad \text{for } 0 \leq y \leq 1,$$

and thus in particular $u \in C^4[0, 1]$. Here are some additional informations on the numerical tests:

- the BDF method of order 3 is chosen;
- numerical experiments with the step sizes $N = 2^q - 1$ for $q = 5, 6, \dots, 11$ are employed;
- for each considered step size h , the noise level $\delta = h^{p+\alpha} = h^{3.5}$ is considered;
- in the numerical experiments, the perturbations are of the form $f_n^\delta = f(x_n) + \Delta_n$ with uniformly distributed random values Δ_n with $|\Delta_n| \leq \delta$;
- in each experiment, the starting value u_0^δ is determined by the strategy described in part (c) of Remark 3.

Table 1. Numerical results

N	δ	$100 * \delta / \ f\ _\infty$	$\max_n u_n^\delta - u(x_n) $	$\max_n u_n^\delta - u(x_n) / \delta^{6/7}$
31	$6.0 * 10^{-6}$	$5.46 * 10^{-4}$	$2.30 * 10^{-3}$	68.5
63	$5.0 * 10^{-7}$	$4.56 * 10^{-5}$	$3.00 * 10^{-4}$	75.1
127	$4.3 * 10^{-8}$	$3.93 * 10^{-6}$	$3.89 * 10^{-5}$	79.7
255	$3.8 * 10^{-9}$	$3.42 * 10^{-7}$	$4.85 * 10^{-6}$	80.5
511	$3.3 * 10^{-10}$	$3.00 * 10^{-8}$	$6.17 * 10^{-7}$	82.3
1023	$2.9 * 10^{-11}$	$2.65 * 10^{-9}$	$7.69 * 10^{-8}$	82.3
2047	$2.6 * 10^{-12}$	$2.33 * 10^{-10}$	$9.69 * 10^{-9}$	83.2

Experiments are employed using the interactive program system Octave (<http://www.octave.org>). The results are shown in Table 1, where $\|f\|_\infty$ denotes the maximum norm of the function f . We conclude this paper with some additional comments on the numerical experiments.

- (a) The relative errors presented in the third column of Table 1 are relatively small.
- (b) Almost the same results as in Table 1 are obtained if all starting values are chosen to be zero, $u_0^\delta = u_1^\delta = u_2^\delta = 0$. This is no surprise since the exact solution of equation (5.12) satisfies $u(0) = u'(0) = u''(0) = 0$.
- (c) Similar numerical experiments were employed with an equation where the solution is of the form $u(y) = e^{-y}(\frac{1}{\Gamma(1.5)}y^{1/2} + \frac{3!}{\Gamma(3.5)}y^{5/2} + \frac{5}{\Gamma(5.5)}y^{9/2})$ for $0 \leq y \leq 1$. Here the ratios $\max_n |u_n^\delta - u(x_n)| / \delta^{6/7}$ deteriorate as N increases. This is no surprise since the solution u does not satisfy the required smoothness condition of Assumption 1.

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