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Nr. 228/1997

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Abstract. We present an extrapolation type algorithm for the numerical solution of fractional order differential equations. It is based on the new result that the sequence of approximate solutions of these equations, computed by means of a recently published algorithm by Diethelm [6], possesses an asymptotic expansion with respect to the stepsize. From this we conclude that the application of extrapolation is justified, and we obtain a very efficient differential equation solver with practically no additional numerical costs. This is also illustrated by a number of numerical examples.

Keywords. Fractional order derivative, fractional order differential equation, quadrature, extrapolation, asymptotic expansion, trapezoidal formula

AMS (MOS) Classification. 26 A 33, 41 A 55, 65 B 05, 65 L 05, 65 L 06, 65 D 30

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0. Introduction and Preliminaries

Recently, differential equations of fractional order have gained very much interest, see for example [6] and the references therein. A prototype example of such a problem is given by the fractional order differential equation

$$(D^q[x - x_0])(t) = \beta x(t) + f(t), \quad 0 \le t \le 1, \tag{0.1}$$

$$x(0) = x_0, \tag{0.2}$$

where f is a prescribed function, $\beta \le 0$, and $D^q x$ denotes the Riemann-Liouville fractional derivative of order $0 < q < 1$ of the function x, defined by (see [18])

$$(D^q x)(t) := \frac{1}{\Gamma(1-q)} \frac{d}{dt} \int_0^t \frac{x(u)}{(t-u)^q} du.$$

An important observation here is (cf. [7]) that we may interchange differentiation and integration to obtain

$$(D^q x)(t) = \frac{1}{\Gamma(-q)} \int_0^t \frac{x(u)}{(t-u)^{q+1}} du,$$

where we now have to interpret the strongly singular integral in Hadamard's finite-part sense. Note that it is a consequence of this identity that we may interpret our equation (0.1) either as a differential equation or as a Volterra integral equation with a strongly singular kernel. Both points of view are justified, and we shall switch between the two interpretations as appropriate.

Following the common practice in the theory of these differential equations, we have incorporated the initial condition (0.2) into the differential equation (0.1). Since the complete initial value problem may easily be transformed to an arbitrary interval, our choice of the interval $[0,1]$ does not mean an essential restriction.

There are very many possible applications for such an equation in areas like mechanical damping laws, diffusion processes, electromagnetics, electrochemistry, material science, the theory of ultra-slow processes, and special functions, see [6,18] and the references therein.

Possible generalizations include the case of non-constant β or nonlinear terms, but these more general equations do not seem to have attracted attention from the point of view of applications so far.

In the present paper, we will mainly focus on equations of the type given in (0.1) and develop an extrapolation algorithm for its numerical solution. In the field of classical, i.e., non-fractional, differential equations, several kinds of extrapolation methods are quite well-developed, see e.g.[11] or [21]. Our aim was to obtain a similar approach to the fractional case.

Extrapolation should be viewed as a numerical process which accelerates the convergence of a given sequence, cf. [2,3,21]. Its applicability depends on the fact that a given sequence of, say, numerical solutions of a discretized differential equation, possesses an asymptotic expansion. For non-fractional differential equations, the first rigorous analysis of this fact was given by Gragg [8,9], and a very nice proof for a general class of methods is due to Hairer & Lubich [10].

In Section 2 of our paper, we prove a corresponding result for the approximate solutions of the equation (0.1), computed by a method recently introduced by Diethelm [6]. This method works as follows: For some $n \in \mathbb{N}$, compute the approximations $\{x_j\}$, $j = 1, \ldots, n$, by the formula

$$x_j = \frac{1}{\alpha_{0j} - (j/n)^q \, \Gamma(-q)\, \beta} \left(\left(\frac{j}{n}\right)^q \Gamma(-q) f(t_j) - \sum_{k=1}^{j} \alpha_{kj} x_{j-k} - \frac{x_0}{q} \right), \tag{0.3}$$

where, for each j, the coefficients α_{kj} are determined by the relation

$$q(1-q) j^{-q} \alpha_{kj} = \begin{cases} -1 & \text{for } k = 0, \\ 2k^{1-q} - (k-1)^{1-q} - (k+1)^{1-q} & \text{for } k = 1, \ldots, j-1. \\ (q-1)k^{-q} - (k-1)^{1-q} + k^{1-q} & \text{for } k = j. \end{cases} \tag{0.4}$$

Then, as shown in [6], each x_j is a good approximation of the true value $x(t_j)$, where $\{t_j\}$ is the equispaced grid on $[0, 1]$. (Here and below, by x_n we always denote the final result of the process (0.3), i.e., the approximation of the value $x(t_n)$.) Note that, due to our assumptions on β and q, the denominator in (0.3) is always strictly negative, and so the numbers x_j are well-defined.

In order to prove our main Theorem 2.1, we first need several results on the existence of an asymptotic expansion for the numerical solution of finite-part integrals by certain numerical methods. In the context of the present paper, these might be viewed as auxiliary results, but it is certainly also interesting by itself, since the numerical methods under consideration are generalizations of the trapezoidal (resp. piecewise constant interpolation) method, and thus the extrapolation process, when applied to these methods, is nothing else but a generalization of the famous Romberg scheme (cf. [19,21]).

Finally, in Section 3 we state the extrapolation process itself, and illustrate its efficiency by means of some numerical examples.

1. Asymptotic Expansions for the Error in Quadrature of Finite Part Integrals

In this section we consider the numerical solution of the Hadamard finite-part integral

$$I_q[g] \;:=\; \int_0^1 t^{-(q+1)} g(t)\, dt\,, \tag{1.1}$$

where $0 < q < 1$ and $g \in C^s[0,1]$ with $q < s$, by means of certain generalized compound quadrature formulae, introduced in [5].

These can be described as follows: Given the equidistant mesh $\{t_j = j/n : j = 0, 1, \ldots, n\}$ on $[0,1]$, and an integer $d \geq 0$, we construct a function g_d that interpolates our function g. On every subinterval $[t_{j-1}, t_j]$ ($j = 1, 2, \ldots, n$), the function g_d is defined to be the dth degree polynomial that interpolates g in the (equidistant) nodes $t_{j-1} + \mu(t_j - t_{j-1})/d$, $\mu = 0, 1, \ldots, d$. (For $d = 0$, we only use the node t_{j-1}.) The piecewise polynomial g_d is then integrated exactly in the finite-part sense with respect to the weight function $t^{-(q+1)}$. Thus, we obtain our desired approximation $Q_n[g] := I_q[g_d]$ with remainder term $R_n := I_q - Q_n$. We remark that, following our construction, it is clear that $Q_n[g]$ depends not only on n but also on the degree d of the piecewise polynomials and on the order q of the singularity. It is possible to use other meshes as well, this has been discussed in [5] too, but for the application we have in mind, the uniform mesh is most appropriate.

First, we are interested in the asymptotic behavior of the so-called Peano error constant

$$\rho \;=\; \rho(s, d, q, R_n) \;:=\; \sup\Big\{ |R_n[g]| \,;\; g \in C^s[0,1] \text{ and } \|g^{(s)}\| \leq 1 \Big\}\,. \tag{1.2}$$

It is well-known (see [5]) that the parameters q, s and d must satisfy the relation

$$q \;<\; s \;\leq\; d + 1\,. \tag{1.3}$$

In [5], asymptotic bounds for $\rho(R_n)$ satisfying (1.3) are given; it is our aim now to analyze further the asymptotic behavior of this quantity in the sense that we establish the existence of an asymptotic expansion. We restrict to the extremal case $s = d + 1$, since this is the only one which will be needed later in Section 2.

Moreover, since $d \in \mathbb{N}_0$ and $q < 1$, (1.3) is automatically satisfied in this case. We therefore may simplify the notation a little bit and write $\rho^{(d)}(R_n)$ instead of $\rho(s, d, q, R_n)$ (note that this notation slightly differs from that used in [5]).

Later, mainly the results for $d = 1$ (trapezoidal formula) will be needed, but for completeness, and also to get the reader used with principle of proof, we begin with the case $d = 0$.

Theorem 1.1: *For $0 < q < 1$, the error constant $\rho^{(0)}(R_n)$ possesses an asymptotic expansion of the form*

$$\rho^{(0)}(R_n) = \frac{-q^{-1}\zeta(q)}{n^{1-q}} + \frac{b_1(q)}{n} + \sum_{\mu=1} \frac{b_{\mu+1}(q)}{n^{2\mu}} \tag{1.4}$$

where the coefficients $b_\mu(q)$ depend on q, but not on n.

Remarks. 1. As usual in the context of asymptotic expansions (cf. [21]), the notation in (1.4) (no upper limit of the sum) denotes the fact that the asymptotic expansion is of arbitrary order, i.e., we have

$$\rho^{(0)}(R_n) = \frac{-q^{-1}\zeta(q)}{n^{1-q}} + \frac{b_1(q)}{n} + \sum_{\mu=1}^{M} \frac{b_{\mu+1}(q)}{n^{2\mu}} + o(n^{-2M}) \tag{1.5}$$

for each $M \in I\!N$.

2. A close inspection of the proof below will show that the coefficients $b_\mu(q)$ can all be given explicitly; but since we are interested in extrapolation methods, the existence of these coefficients is information enough.

3. Since $\zeta(q)$ is negative for $0 < q < 1$, the asymptotic constant $-q^{-1}\zeta(q)$ is indeed positive. Furthermore, in connection with [5], Theorem 2.2, we obtain the inclusion

$$\frac{(q+1)/2}{(1-q)q} - \frac{1}{6} < \frac{-\zeta(q)}{q} < \frac{(q+1)/2}{(1-q)q} .$$

Proof of Theorem 1.1. In [5], Theorem 2.2, is was shown that

$$\begin{aligned} \rho^{(0)}(R_n) &= \frac{n^{q-1}}{(1-q)q}\left(n^{1-q} - (1-q)\cdot\sum_{\nu=1}^{n}\nu^{-q}\right) \\ &= \frac{1}{(1-q)q}\left(1 - (1-q)\cdot n^{q-1}\cdot\sum_{\nu=1}^{n}\nu^{-q}\right) . \end{aligned} \tag{1.6}$$

Since $\sum_{\nu=1}^{n}\nu^{-q}$ is the n^{th} partial sum of the Riemann $\zeta-$ function, we obtain the existence of the asymptotic expansion (cf. [17,21])

$$n^{q-1}\cdot\sum_{\nu=1}^{n}\nu^{-q} = n^{q-1}\zeta(q) - \frac{1}{q-1} + \frac{1}{2n} + \sum_{\mu=1}\frac{\gamma_\mu(q)}{n^{2\mu}} \tag{1.7}$$

with certain coefficients γ_μ. Inserting (1.7) into (1.6), gives

$$\begin{aligned} \rho^{(0)}(R_n) &= \frac{1}{(1-q)q}\left(1 - \frac{(1-q)\cdot\zeta(q)}{n^{1-q}} - 1 - \frac{1-q}{2n} - \sum_{\mu=1}\frac{(1-q)\,\gamma_\mu(q)}{n^{2\mu}}\right) \\ &= \frac{-\zeta(q)}{q\cdot n^{1-q}} - \frac{1}{2qn} + \sum_{\mu=1}\frac{-q^{-1}\gamma_\mu(q)}{n^{2\mu}} , \end{aligned}$$

which is of the desired form. $\square$

Applying the same methods, in a bit more tricky way, as in the proof of Theorem 1.1, we obtain an analoguous result for $\rho^{(1)}(R_n)$, i.e., for the application of the modified trapezoidal rule. This will be the basis for the proof of our main result in the next section, the existence of an asymptotic expansion for the fractional differential equation solver described in Section 0.

Also, the remarks following the formulation of Theorem 1.1 carry over to the following result.

Theorem 1.2: *For $0 < q < 1$, the error constant $\rho^{(1)}(R_n)$ possesses an asymptotic expansion of the form*

$$\rho^{(1)}(R_n) = \frac{-2\,\zeta(q-1)}{q\,(1-q)} \cdot \frac{1}{n^{2-q}} + \sum_{\mu=1} \frac{c_\mu(q)}{n^{2\mu}} \tag{1.8}$$

where the coefficients $c_\mu(q)$ depend on q, but not on n.

Proof. Again we refer to [5], where it was shown that $\rho^{(1)}(R_n)$ can be decomposed into the sum

$$\rho^{(1)}(R_n) := r_1(n,q) + r_2(n,q) + r_3(n,q) \tag{1.9}$$

with

$$\begin{aligned} r_1(n,q) &= \frac{n^{q-2}-1}{2-q}, \\ r_2(n,q) &= \frac{n^{q-2}}{(1-q)q}\left((q+1)n^{2-q} + n^{1-q} - q - 2 \cdot \sum_{\nu=1}^{n} \nu^{1-q}\right), \quad \text{and} \\ r_3(n,q) &= \frac{n^{q-2}}{(1-q)(2-q)}. \end{aligned}$$

Now we have to manipulate these terms and to collect the coefficients of the resulting asymptotic expansions. First we get that

$$r_1(n,q) + r_3(n,q) = \frac{n^{q-2}}{1-q} - \frac{1}{2-q}. \tag{1.10}$$

Then, applying (1.7) we obtain

$$\begin{aligned} r_2(n,q) &= \frac{q+1}{(1-q)q} + \frac{1}{(1-q)qn} - \frac{n^{q-2}}{1-q} - \frac{2\,n^{q-2}}{(1-q)q} \cdot \sum_{\nu=1}^{n} \nu^{1-q} \\ &= \frac{q+1}{(1-q)q} + \frac{1}{(1-q)qn} - \frac{n^{q-2}}{1-q} - \frac{2\,n^{q-2}}{(1-q)q} \cdot \zeta(q-1) + \\ &\quad + \frac{2}{(q-2)(1-q)q} - \frac{1}{(1-q)qn} + \sum_{\mu=1} \frac{\widetilde{\gamma}_\mu(q)}{n^{2\mu}} \\ &= \frac{(q-2)(q+1)+2}{(q-2)(1-q)q} - \left(\frac{1}{1-q} + \frac{2\,\zeta(q-1)}{(1-q)q}\right) n^{q-2} + \sum_{\mu=1} \frac{\widetilde{\gamma}_\mu(q)}{n^{2\mu}} \end{aligned} \tag{1.11}$$

with coefficients $\widetilde{\gamma}_\mu(q)$, which do not depend on n.

Now we sum up the right hand sides of (1.10) and find that the constant term cancels out, while the coefficient of n^{q-2} equals $\frac{-2\zeta(q-1)}{(1-q)q}$. This completes the proof of Theorem 1.2. □

We now prove the main result of this section, Theorem 1.3, on the existence of an asymptotic expansion for the remainder itself, provided that the function g is smooth enough:

Theorem 1.3: *If, for some $m \geq 1$, $g \in C^{m+1}[0,1]$, then the sequence of remainders $R_n[g]$ possesses the asymptotic expansion*

$$R_n[g] = \sum_{\mu=2}^{m+1} d_\mu n^{q-\mu} + \sum_{\mu=1}^{\mu^*} d^*_\mu n^{-2\mu} + O(n^{-m-1+q}) \qquad \text{for } n \to \infty \tag{1.12}$$

where μ^* is the integer satisfying $2\mu^* < m+1-q < 2(\mu^*+1)$, and d_μ and d^*_μ are certain coefficients that depend on g.

Proof. The first steps of the proof follow the ideas of [12], Section 2. By construction of the quadrature formula, we can represent the integration error in the form

$$\begin{aligned} R_n[g] \;&=\; \frac{1}{n}\sum_{l=0}^{n-1}\int_0^1 ((l+s)/n)^{-q-1}\cdot \\ &\quad \cdot \Big([g((l+s)/n) - g(l/n)](1-s) + [g((l+s)/n) - g((l+1)/n)]s\Big)\,ds\,. \end{aligned}$$

We express the two terms in brackets with the help of Taylor's expansion centered at $(l+s)/n$ and obtain

$$R_n[g] = \frac{1}{n}\sum_{l=0}^{n-1}\int_0^1 ((l+s)/n)^{-q-1}\left(\sum_{r=0}^{m-2} n^{-r-2}g^{(r+2)}((l+s)/n)s(1-s)\pi_r(s) + \epsilon_l(s)\right)ds$$

where $\pi_r(s) = (s^{r+1} - (s-1)^{r+1})/(r+2)!$ is a polynomial of degree r and ϵ_l is the error of the Taylor approximation. Using Lagrange's representation of the latter, it is easily seen that

$$R_n[g] = \frac{1}{n}\sum_{l=0}^{n-1}\int_0^1 ((l+s)/n)^{-q-1}\sum_{r=0}^{m-2} n^{-r-2}g^{(r+2)}((l+s)/n)s(1-s)\pi_r(s)ds + O(n^{-m-1+q}).$$

Reorganization of the double sum yields

$$R_n[g] = \sum_{r=0}^{m-2} n^{-r-2}\int_0^1 s(1-s)\pi_r(s)n^{-1}\sum_{l=0}^{n-1}((l+s)/n)^{-q-1}g^{(r+2)}((l+s)/n)ds + O(n^{-m-1+q}).$$

This expression has got a form that allows a direct application of Theorem 3.2 of [16]. As a consequence of this, we derive

$$R_n[g] = \sum_{r=0}^{m-2} n^{-r-2}\left(\sum_{j=0}^{m-r-1} a_{j,r}n^{q-j} + \sum_{j=0}^{m-r-1} b_{j,r}n^{-j} + O(n^{r-m})\right) + O(n^{-m-1+q})$$

where, in particular, the coefficients $b_{j,r}$ are given by

$$\text{const.} \int_0^1 s(1-s)\pi_r(s)B_j(s)ds$$

where B_j is the j th Bernoulli polynomial. It is easily seen that π_r is an even (odd) function with respect to the point $1/2$ if r is even (odd). The same is known about the Bernoulli polynomial. Thus, the integral vanishes if $r+j$ is odd, and therefore the expansion does not contain any odd integer powers of n. Collecting terms with identical powers of n in the rest of the last expression, we obtain (1.12). □

A numerical example, which illustrates the statement of Theorem 1.3 quite nicely, is given in Section 3 (cf. Table 2).

We conclude this section by establishing some results on the Peano kernels of the remainder functional R_n. The principles are similar to those applied to the classical trapezoidal method, see, e.g., Sections II.2 and V.1 of [1]. However, in the classical case the analysis is drastically simplified by various properties like symmetry and periodicity of the kernel functions defined below that do not hold in our situation.

Lemma 1.4: *Let* $D_1(x) := R_n[(\cdot - x)_+^0]$ *for* $0 < x < 1$, *and* $D_1(0) := D_1(1) := 0$, *where* $(\cdot)_+^0$ *is the truncated power function given by*

$$x_+^0 := \begin{cases} 0 & \text{for } x < 0, \\ 1/2 & \text{for } x = 0, \\ 1 & \text{for } x > 0. \end{cases}$$

Then, for every $g \in C^1[0,1]$,

$$R_n[g] = \int_0^1 D_1(x)g'(x)dx. \tag{1.13}$$

Proof. This is a simple consequence of the classical Peano kernel theorem [20]. □

The function D_1 introduced in Lemma 1.4 is usually called the first Peano kernel of the remainder functional R_n. Based on this function, we shall now define the functions D_k, $k = 2, 3, \dots$, by the relations

$$D_k'(x) = D_{k-1}(x) \tag{1.14}$$

and

$$\int_0^1 D_k(x)dx = 0. \tag{1.15}$$

Since $R_n[g] = 0$ for $g(x) = x$, it follows from the Peano kernel theory that (1.15) also holds for $k = 1$.

Lemma 1.5: *Let* $g \in C^k[0,1]$ *for some* $k \geq 1$ *. Then,*

$$R_n[g] = (-1)^{k+1} \int_0^1 D_k(x) g^{(k)}(x)dx + \sum_{j=1}^{k-1} (-1)^{j+1} D_{j+1}(0) \left(g^{(j)}(1) - g^{(j)}(0) \right). \quad (1.16)$$

Proof. We note that, as a consequence of (1.14) and (1.15),

$$D_k(1) = D_k(0) \quad \text{for } k = 1, 2, \dots .$$

Thus, (1.16) follows from (1.13) by $(k-1)-$ fold partial integration. □

Lemma 1.6: *For* $k = 2, 3, \dots$, *we have the asymptotic expansions*

$$D_k(0) = \sum_{\mu=2}^{k} \gamma^*_{\mu,k} n^{q-\mu} + \sum_{\mu=1} \gamma_{\mu,k} n^{-2\mu}$$

with some constants $\gamma_{\mu,k}$ *and* $\gamma^*_{\mu,k}$ *. In particular,* $\gamma^*_{k,k} \neq 0$ *.*

Proof. We note that, as a consequence of (1.14) and (1.15),

$$D_k(0) = \int_0^1 t D_{k-1}(t) dt.$$

Performing $k-2$ partial integrations and using (1.14) and $D_j(1) = D_j(0)$ (cf. the proof of Lemma 1.5), we obtain

$$D_k(0) = \frac{(-1)^k}{(k-1)!} \int_0^1 t^{k-1} D_1(t) dt + \sum_{j=1}^{k-2} \frac{(-1)^{j+1}}{(j+1)!} D_{k-j}(0).$$

Using (1.13), we derive

$$D_k(0) = \frac{(-1)^k}{k!} R_n[p_k] + \sum_{j=1}^{k-2} \frac{(-1)^j}{j!} D_{k-j}(0)$$

where $p_k(x) = x^k$.

In the case $k = 2$, we note that from a remark in [5], p. 487, $R_n[p_2] = -2\rho^{(1)}(R_n)$, so an application of (1.8) completes the proof in this case.

For $k \geq 3$, we can see that, by construction,

$$R_n[p_k] = \sum_{\nu=1}^{n} \int_{(\nu-1)/n}^{\nu/n} t^{-q-1} \left[t^k - n^{1-k}(\nu^k - (\nu-1)^k)t - n^{-k}(\nu^k - \nu^{k+1} + \nu(\nu-1)^k) \right] dt.$$

A simple explicit calculation yields that this can be rearranged to

$$R_n[p_k] = \frac{1}{k-q} - \frac{n^{q-k}}{1-q} S_1 + \frac{n^{q-k}}{q} S_2$$

where

$$S_1 = \sum_{\nu=1}^{n} (\nu^k - (\nu-1)^k)(\nu^{1-q} - (\nu-1)^{1-q})$$

and

$$S_2 = \sum_{\nu=2}^{n} (\nu^k - \nu^{k+1} + \nu(\nu-1)^k)(\nu^{-q} - (\nu-1)^{-q}).$$

We notice that we can reorganize S_1 in a form that admits an application of classical extrapolation methods [21]. A rather long but straightforward calculation then yields

$$n^{q-k} S_1 = \frac{k(1-q)}{k-q} + \phi_k n^{q-k} + \sum_{\mu=1} \psi_{\mu,k} n^{-2\mu}.$$

where $\psi_{\mu,k}$ are certain coefficients that can be determined explicitly and

$$\phi_k = -2 \sum_{\substack{j=0 \\ j-k \text{ odd}}}^{k-2} \binom{k}{j} \zeta(q-j-1)$$

is a nonzero constant.

In a similar fashion, we can see that

$$n^{q-k} S_2 = \frac{(k-1)q}{k-q} - \phi_k n^{q-k} + \sum_{\mu=1} \psi^*_{\mu,k} n^{-2\mu}$$

where again the coefficients $\psi^*_{\mu,k}$ can be determined explicitly and ϕ_k is as in the previous expression. Adding up these partial results, the lemma follows. □

We remark that, by using methods similar to that in the proof of Lemma 1.6, one can also prove the existence of an asymptotic expansion for the term

$$\int_0^1 D_k(x) g^{(k)}(x) dx\,,$$

and so, by means of Lemma 1.5, give a new proof of Theorem 1.3.

2. Asymptotic Expansions for the Numerical Solution of Fractional Order Differential Equations

The method described by (0.3) is obtained by replacing the finite-part integral in the Volterra interpretation of (0.1) by a product trapezoidal quadrature formula, see [6] for the details. Thus, if we look at (0.1) as a hypersingular Volterra equation, the method should be called a product trapezoidal method. On the other hand, if we prefer the differential equation interpretation of (0.1), the method corresponds to the two-point backward differentiation formula, cf. [15].

We shall now derive an asymptotic expansion of the error of this method. Based on this expansion, we shall give an extrapolation method in Section 3.

Theorem 2.1: *Let, for $n \in \mathbb{N}$, x_n denote the final result of the process (0.3), and suppose that the function f (and therefore x) is sufficiently smooth.*

Then there exist coefficients $c_\mu = c_\mu(q)$ and $c_\mu^* = c_\mu^*(q)$ such that the sequence $\{x_n\}$ possesses an asymptotic expansion of the form

$$x_n = x(t_n) + \sum_{\mu=2}^{M_1} c_\mu n^{q-\mu} + \sum_{\mu=1}^{M_2} c_\mu^* n^{-2\mu} + o(n^{-M_3}) \quad \textit{for } n \to \infty \tag{2.1}$$

where M_1 and M_2 depend on the smoothness of x (resp. f), and

$$M_3 = \min\{q - M_1, 2M_2\} .$$

Proof. In order to prove Theorem 2.1, we have to consider the asymptotic behaviour of $x(t_j) - x_j$, $j = 1, \ldots, n$, for $j \to \infty$. Clearly, this only makes sense if the location of the point t_j remains fixed, i.e., we investigate the differences

$$\epsilon_j := x(t_j) - x_j \quad \text{for } j \to \infty, \quad \text{with } jh \text{ is constant,} \tag{2.2}$$

where h is the stepsize. In other words, there is a constant c, independent of n, such that

$$j = c \cdot n , \tag{2.3}$$

and consequently, we see that if one of the sequences under consideration possesses an asymptotic expansion w.r.t. j, it possesses at the same time one w.r.t. n, and vice versa. Taking this into account, we now claim that, for each fixed j, the difference ϵ_j possesses an asymptotic expansion of the type given in (2.1), i.e.,

$$\epsilon_j = \sum_{\mu=2}^{N_1} \tilde{c}_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2} \tilde{c}_\mu^* n^{-2\mu} + o(n^{-N_3}) \quad \text{for } j \to \infty . \tag{2.4}$$

This can be seen as follows: Introducing, as in [6], the auxiliary function $\Psi_j(t) := x(t_j - t_j t) - x(0)$, it can be shown in a straightforward manner (cf. [6]) that

$$f(t_j) + \beta x(t_j) = \frac{t_j^{-q}}{\Gamma(-q)} \left(\sum_{k=0}^{j} \alpha_{kj} (x(t_{j-k}) - x(0)) + R_j[\Psi_j] \right) . \tag{2.5}$$

Using the fact that

$$\sum_{k=0}^{j} \alpha_{kj} = \frac{-1}{q} , \tag{2.6}$$

it follows from (2.5) in combination with (0.3) and (2.3) that

$$\begin{aligned} \epsilon_j &= \frac{1}{\alpha_{0j} - (j/n)^q\,\Gamma(-q)\,\beta}\left(-\sum_{k=1}^{j}\alpha_{kj}(x(t_{j-k}) - x_{j-k}) - R_j[\Psi_j]\right) \\ &= \frac{1}{c^q\,\Gamma(-q)\,\beta - \alpha_{0j}}\left(\sum_{k=1}^{j}\alpha_{kj}\epsilon_{j-k} + R_j[\Psi_j]\right) . \end{aligned} \tag{2.7}$$

Since the function x was assumed to be smooth enough, the derivatives of the function Ψ_j exist and thus we find that, for $\nu \geq 1$ and all $t \in [0,1]$,

$$\Psi_j^{(\nu)}(t) = (-t_j)^\nu \cdot x^{(\nu)}(t_j - t_j t) ,$$

and so, with (2.3),

$$\Psi_j^{(\nu)}(0) = (-c)^\nu \cdot x^{(\nu)}(c) \quad \text{and} \quad \Psi_j^{(\nu)}(1) = (-c)^\nu \cdot x^{(\nu)}(0) . \tag{2.8}$$

Therefore, we obtain from (1.12) that the remainder terms $R_j[\Psi_j]$ possess expansions of the form

$$R_j[\Psi_j] = \sum_{\mu=2}^{\tilde{M}_1} d_\mu j^{q-\mu} + \sum_{\mu=1}^{\tilde{M}_2} d_\mu^* j^{-2\mu} + O(j^{-\tilde{M}_1-1+q}) \quad \text{for } j \to \infty \tag{2.9}$$

with coefficients depending on x, but neither on j nor on n, and $\tilde{M}_1$ and $\tilde{M}_2$ depending on the smoothness of x (resp. f).

We now use (2.7) in order to complete the proof of (2.4). Since $\epsilon_0 = 0$, the assertion for $j = 1$ follows directly from (2.9). Now let $j \geq 2$, and assume that (2.4) holds true for $\epsilon_1, \ldots, \epsilon_{j-1}$.

Starting from (2.7), and using relations (2.4), (2.6) and (2.9), we obtain successively

$$\begin{aligned} \epsilon_j &= \frac{1}{c^q\,\Gamma(-q)\,\beta - \alpha_{0j}}\left(\sum_{k=1}^{j}\alpha_{kj}\epsilon_{j-k} + R_j[\Psi_j]\right) \\ &= \frac{1}{c^q\,\Gamma(-q)\,\beta - \alpha_{0j}}\left(\left(\sum_{\mu=2}^{N_1}\tilde{c}_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2}\tilde{c}_\mu^* n^{-2\mu} + o(n^{-N_3})\right)\left(\sum_{k=0}^{j}\alpha_{kj} - \alpha_{0j}\right) + R_j[\Psi_j]\right) \end{aligned}$$

and so

$$\begin{aligned} (\alpha_{0j} - c^q\,\Gamma(-q)\,\beta)\cdot\epsilon_j = {} & \frac{1}{q}\cdot\left(\sum_{\mu=2}^{N_1}\tilde{c}_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2}\tilde{c}_\mu^* n^{-2\mu} + o(n^{-N_3})\right) + \\ & + \sum_{\mu=2}^{\tilde{M}_1}\tilde{d}_\mu n^{q-\mu} + \sum_{\mu=1}^{\tilde{M}_2}\tilde{d}_\mu^* n^{-2\mu} + O(n^{-\tilde{M}_1-1+q}) + \\ & + \alpha_{0j}\cdot\left(\sum_{\mu=2}^{N_1}\tilde{c}_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2}\tilde{c}_\mu^* n^{-2\mu} + o(n^{-N_3})\right) . \end{aligned} \tag{2.10}$$

Rearranging this according to powers of n and remembering that $\alpha_{0j} = -q(1-q)j^q = q(q-1)(nc)^q$, we see that (2.10) is of the form

$$\begin{aligned}\left(n^q + \frac{\Gamma(-q)\,\beta}{q(1-q)}\right)\cdot \epsilon_j \;&=\; \sum_{\mu=2}^{\tilde N_1} \tilde e_\mu n^{q-\mu} + \sum_{\mu=1}^{\tilde N_2} \tilde e^*_\mu n^{-2\mu} + o(n^{-\tilde N_3}) \;+ \\ &\quad + \; n^q\cdot\left(\sum_{\mu=2}^{N_1} \hat c_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2} \hat c^*_\mu n^{-2\mu} + o(n^{-N_3})\right)\,.\end{aligned} \tag{2.11}$$

This already shows that the sequence $\{\epsilon_j\}$ possesses an asymptotic expansion w.r.t. powers of n, say

$$\epsilon_j \;=\; \sum_{\mu=1}^{M} \gamma_\mu\cdot n^{-\rho_\mu} \;+ o(n^{-\rho_M})\,. \tag{2.12}$$

with

$$0 \;<\; \rho_1 \;<\; \rho_2 \;<\; \cdots\,.$$

Thus we obtain the relation

$$\begin{aligned}&\left(n^q + \frac{\Gamma(-q)\,\beta}{q(1-q)}\right)\cdot\left(\sum_{\mu=1}^{M} \gamma_\mu\cdot n^{-\rho_\mu} \;+ o(n^{-\rho_M})\right) \;= \\ &= \sum_{\mu=2}^{\tilde N_1} \tilde e_\mu n^{q-\mu} + \sum_{\mu=1}^{\tilde N_2} \tilde e^*_\mu n^{-2\mu} + o(n^{-\tilde N_3}) \;+\; n^q\cdot\left(\sum_{\mu=2}^{N_1} \hat c_\mu n^{q-\mu} + \sum_{\mu=1}^{N_2} \hat c^*_\mu n^{-2\mu} + o(n^{-N_3})\right),\end{aligned} \tag{2.13}$$

and we have to compare the exponents of n in (2.13). Since the largest ones on both sides must be identical, we get at once $2q-2 = q-\rho_1$, hence

$$\rho_1 \;=\; 2-q\,.$$

(This means that the sequence $\{\epsilon_j\}$ converges like n^{q-2} and is inasmuch a result already known from [6]).

We now claim that

$$q-\rho_2 \;=\; -\rho_1\,.$$

Assume to the contrary that $q-\rho_2 > -\rho_1 (= q-2)$. Since $-2 < q-2$, and because $q-\rho_2$ is equal to one of the exponents on the right hand side of (2.13), it follows that $q-\rho_2 = 2q-3$. Hence $\rho_2 = 3-q$, which is a contradiction to the fact that $3-q > 2$.

Now assume that $q-\rho_2 < -\rho_1$. Under this assumption it is clear that $q-\rho_2$ cannot be equal to $q-2$. So it follows that $q-\rho_2 = -2$, hence $\rho_2 = 2+q$. But then, as above, $2+q$ must appear as an exponent on the right hand side of (2.13), and this implies that $2+q = 3-2q$, which is impossible, except for the case $q = 1/3$. Excluding this for the moment, we have shown that $q - \rho_2 = -\rho_1 = q - 2$, hence

$$\rho_2 = 2.$$

If $q = 1/3$, then either $q - \rho_3 = q - 3$ or $q - \rho_3 = 2q - 3$. In the first case it follows that

$$-\rho_3 = -3 = 2q - 4 = \frac{2}{3} - 4,$$

which is wrong. In the second case, we get that $\rho_3 = 3 - q$, which in turn implies that $\rho_2 = 2$.

In any case we have shown that (at least) the first two exponents in the asymptotic expansion in (2.4) are correct. Now we proceed by comparing the next pairs of exponents and obtain, after some laborious but straightforward case distinctions the desired equalities of exponents. It follows that ϵ_j is of the form claimed in (2.4), and, after setting $j = n$ and some obvious re-labeling, the proof of Theorem 2.1 is complete. □

3. The Extrapolation Algorithm and Numerical Examples

Having proved the existence of the asymptotic expansion (2.1) (resp. (1.12)), we are now able to state an extrapolation algorithm for the numerical solution of the initial value problem (0.1), (0.2), since it is just a special case of the general so-called logarithmic extrapolation process (or repeated Richardson extrapolation), as described for example in [21].

We recall from (2.1) that the approximations x_n possess an asymptotic expansion, which we now write for convenience in the form

$$x_n = x(t_n) + \sum_{\mu=1}^{M} \gamma_\mu n^{-\lambda_\mu} + o(n^{-\lambda_M}) \quad \text{for } n \to \infty$$

where, for $j = 1, 2, \ldots$,

$$\lambda_{3j} = 2j + 1 - q, \qquad \lambda_{3j-1} = 2j, \qquad \text{and } \lambda_{3j-2} = 2j - q. \tag{3.1}$$

Now, choose natural numbers n_0, b (usually, $b = 2$), and K with $K \leq M$, and compute by the method (0.3) the sequence of numerical solutions

$$y_i^{(0)} := x_{n_i}, \qquad i = 0, 1, 2 \ldots, \tag{3.2}$$

where $n_i := n_0 \cdot b^i$ for all i.

The algorithm is now to apply *linear extrapolation* , i.e., to compute the sequences of improved numerical solutions

$$y_i^{(k)} := y_{i+1}^{(k-1)} + \frac{y_{i+1}^{(k-1)} - y_i^{(k-1)}}{b^{\lambda_k} - 1}, \quad \begin{cases} k = 1, 2, \ldots, K, \\ i = 0, 1, \ldots, \end{cases} \tag{3.3}$$

with the λ_k 's defined in (3.1).

Then each of the sequences $\{y_i^{(k)}\}_{i\in\mathbb{N}}$ possesses an asymptotic expansion of the form

$$y_i^{(k)} = x(t_n) + \sum_{\mu=k+1}^{M} \gamma_\mu^{(k)} \cdot n_i^{-\lambda_\mu} + o(n_i^{-\lambda_M}) \quad \text{for } n_i \to \infty$$

with coefficients $\gamma_\mu^{(k)}$, which are independent of n_i .

In particular, each of the sequences $\{y_i^{(k)}\}$ converges like $n_i^{-\lambda_{k+1}}$ and thus faster to the limit $x(t_n)$ than its predecessor.

For the application of the method, it is of course important to investigate the stability of the method. In this context, we have the following positive result.

Theorem 3.1: *For arbitrary K , the method given by (3.2), (3.3) for the approximate calculation of $x(1)$ is stable.*

Proof. For $K = 0$, i.e. the basic algorithm without extrapolation, this result is due to Lubich [15]. For $K > 0$, we can see that the final result is obtained by a finite linear combination of non-extrapolated values. Since the latter have already been shown to be the result of a stable process, the overall extrapolation process is also stable. □

The argumentation used in the proof of Theorem 3.1 is essentially identical to the one used in the classical case of differential equations of integer order, see, e.g., [13], section 5.3, or [21].

Note that the computational costs of the process (3.3) is very, very low, compared to the that of the algorithm (0.3) itself (since (3.3) is a completely linear process), but that the improvement of the accuracy is significant, as we will show now by some numerical examples. The results (and similary the errors) of the extrapolation process (3.3) are usually displayed in a triangular array of the following form, called *Romberg tableau*.

$$\begin{array}{ccccc}
y_0^{(0)} & & & & \\
 & y_0^{(1)} & & & \\
y_1^{(0)} & & \ddots & & \\
 & \vdots & & y_0^{(K-1)} & \\
\vdots & & \vdots & & y_0^{(K)} \\
 & \vdots & & y_1^{(K-1)} & \vdots \\
\vdots & & \cdot^{\cdot^{\cdot}} & \vdots & \\
 & y_{K-1}^{(1)} & \vdots & & \\
y_K^{(0)} & \vdots & & & \\
\vdots & & & &
\end{array}$$

Table 1. A Romberg Tableau

We conclude our paper by giving the results of some numerical tests. In all cases we have chosen $b = 2$ and $n_0 = 10$, i.e., our sequence n_i is given by

$$n_i = 10 \cdot 2^i, \qquad i = 0, 1, 2 \ldots .$$

Our first example is an illustration of Theorem 1.3. We consider the case $g(x) = \exp(1 - x)$. An explicit calculation yields $\int_0^1 x^{-q-1} g(x) dx = -{}_1F_1(1; 1 - q; 1)/q$. We calculated some approximations for this integral using our quadrature formula for various values of n, and then established the corresponding Romberg tableau for the quadrature errors $R_{n_i}[g]$. For the sake of brevity, we only state the tableau for $q = 1/2$ here explicitly; for all other choices of q, we obtained analoguous results.

-6.22(-2)								
	-1.57(-3)							
-2.30(-2)		1.97(-5)						
	-3.79(-4)		3.82(-7)					
-8.38(-3)		3.80(-6)		1.44(-9)				
	-9.18(-5)		3.51(-8)		-8.67(-12)			
-3.02(-3)		7.01(-7)		8.17(-11)		-1.80(-14)		
	-2.24(-5)		3.18(-9)		-4.00(-13)		-5.20(-17)	
-1.08(-3)		1.27(-7)		4.73(-12)		-4.49(-16)		1.15(-20)
	-5.51(-6)		2.85(-10)		-1.81(-14)		-8.01(-19)	
-3.86(-4)		2.26(-8)		2.79(-13)		-1.07(-17)		
	-1.36(-6)		2.55(-11)		-8.11(-16)			
-1.38(-4)		4.02(-9)		1.67(-14)				
	-3.37(-7)		2.27(-12)					
-4.88(-5)		7.12(-10)						
	-8.37(-8)							
-1.73(-5)								

Table 2. Quadrature Errors for $g(x) = \exp(1 - x)$.

Note that we have adopted the notation $-6.22(-2)$ to stand for $-6.22 \cdot 10^{-2}$, etc. The power of the extrapolation method is clearly exhibited: For example, using only one extrapolation step based on formulas with 81 and 161 nodes, the results are better than those obtained without extrapolation with 1281 nodes. The use of more extrapolation steps gives even better results. Furthermore, the asymptotic expansion of Theorem 1.3 is nicely recovered in this table. It is seen that the values in the columns converge to zero with the convergence order described by Theorem 1.3: The first column converges as n^{q-2}, the second as n^{-2}, and the following columns as n^{q-3}, n^{q-4}, n^{-4}, n^{q-5}, n^{q-6}, and n^{-6}, respectively.

We now come to examples illustrating the algorithm for the numerical solution of the differential equation itself. We tested the algorithm using various differential equations. All tests were performed with five different values for q, namely $q = 1/10$, $q = 1/4$, $q = 1/2$, $q = 3/4$, and $q = 9/10$. In the following we show a representative selection of our results.

Example 1: As a first example, we looked at the differential equation

$$(D^q x)(t) + x(t) = t^2 + \frac{2}{\Gamma(3-q)} t^{2-q}, \quad x(0) = 0,$$

whose exact solution is given by

$$x(t) = t^2.$$

This problem has already been considered in [6]. We displayed the errors of the basic algorithm and of the first two extrapolation steps in the Romberg tableau. In all cases of q under consideration, we can observe that the first column (the errors of the basic algorithm without extrapolation) converges as n^{q-2}. The second column (errors using one extrapolation step) converges as n^{-2}, and the last column (two extrapolation steps) converges as n^{q-3}. As an example, we show in Table 3 the results for $q = 1/10$ and $q = 1/2$.

-5.53(-4)		
	-1.99(-5)	
-1.63(-4)		1.18(-8)
	-4.97(-6)	
-4.73(-5)		1.47(-9)
	-1.24(-6)	
-1.36(-5)		1.87(-10)
	-3.10(-7)	
-3.86(-6)		2.43(-11)
	-7.75(-8)	
-1.09(-6)		3.19(-12)
	-1.94(-8)	
-3.07(-7)		4.22(-13)
	-4.84(-9)	
-8.57(-8)		5.60(-14)
	-1.21(-9)	
-2.39(-8)		

Table 3a. Example 1, $q = 1/10$.

-7.72(-3)		
	-1.30(-4)	
-2.82(-3)		1.91(-6)
	-3.11(-5)	
-1.02(-3)		2.95(-7)
	-7.56(-6)	
-3.64(-4)		4.68(-8)
	-1.86(-6)	
-1.30(-4)		7.63(-9)
	-4.58(-7)	
-4.62(-5)		1.27(-9)
	-1.14(-7)	
-1.64(-5)		2.14(-10)
	-2.82(-8)	
-5.82(-6)		3.67(-11)
	-7.03(-9)	
-2.06(-6)		

Table 3b. Example 1, $q = 1/2$.

Example 2: The second example is the differential equation

$$(D^q x)(t) + x(t) = t^4 - \frac{1}{2}t^3 - \frac{3}{\Gamma(4-q)}t^{3-q} + \frac{24}{\Gamma(5-q)}t^{4-q}, \quad x(0) = 0,$$

whose exact solution is given by

$$x(t) = t^4 - \frac{1}{2}t^3.$$

In all cases of q under consideration, we can observe that the first column (the errors of the basic algorithm without extrapolation) converges exactly as n^{q-2}, and the second column (errors using one extrapolation step) as n^{-2}. This is well in line with the results of Section 2. For the third column (two extrapolation steps), we have the effect that for $q \leq 1/2$, we have a convergence rate of exactly n^{q-3} (cf. Table 4a), while for example for $q = 9/10$, the convergence seems to be even a bit faster.

-5.64(-3)		
	-3.17(-4)	
-1.90(-3)		3.30(-6)
	-7.67(-5)	
-6.18(-4)		6.03(-7)
	-1.87(-5)	
-1.97(-4)		1.00(-7)
	-4.60(-6)	
-6.18(-5)		1.59(-8)
	-1.14(-6)	
-1.92(-5)		2.46(-9)
	-2.83(-7)	
-5.90(-6)		3.74(-10)
	-7.05(-8)	
-1.80(-6)		5.64(-11)
	-1.76(-8)	
-5.48(-7)		

Table 4a. Example 2, $q = 1/4$.

-7.70(-2)		
	-1.00(-3)	
-3.65(-2)		-7.07(-5)
	-3.03(-4)	
-1.72(-2)		-1.76(-5)
	-8.90(-5)	
-8.06(-3)		-4.03(-6)
	-2.53(-5)	
-3.77(-3)		-8.85(-7)
	-6.98(-6)	
-1.76(-3)		-1.89(-7)
	-1.89(-6)	
-8.24(-4)		-3.99(-8)
	-5.02(-7)	
-3.85(-4)		-8.31(-9)
	-1.32(-7)	
-1.80(-4)		

Table 4b. Example 2, $q = 9/10$.

Example 3: The third example, the differential equation

$$(D^q(x-1))(t) + 2x(t) = 2\cos\pi t + \frac{t^{-q}}{2\Gamma(1-q)}({}_1F_1(1; 1-q; i\pi t) + {}_1F_1(1; 1-q; -i\pi t) - 2),$$
$$x(0) = 1,$$

with exact solution

$$x(t) = \cos\pi t,$$

is also taken from [6]. Once more, in all cases of q under consideration, we find convergence as n^{q-2} in the first and n^{-2} in the second column. The figures in the last column give, at least for $q \le 1/2$, a hint towards a convergence rate of n^{q-3}. For larger values of q, however, it seems that one must go much further along the sequence before the asymptotic behaviour really sets in.

-4.48(-3)		
	-2.34(-4)	
-1.50(-3)		3.12(-6)
	-5.61(-5)	
-4.84(-4)		3.42(-7)
	-1.38(-5)	
-1.54(-4)		3.81(-8)
	-3.41(-6)	
-4.81(-5)		4.41(-9)
	-8.50(-7)	
-1.49(-5)		5.36(-10)
	-2.12(-7)	
-4.57(-6)		6.87(-11)
	-5.30(-8)	
-1.40(-6)		9.20(-12)
	-1.32(-8)	
-4.25(-7)		

Table 5a. Example 3, $q = 1/4$.

-1.57(-2)		
	-7.47(-4)	
-6.04(-3)		1.77(-5)
	-1.73(-4)	
-2.25(-3)		2.93(-6)
	-4.12(-5)	
-8.21(-4)		4.56(-7)
	-9.95(-6)	
-2.97(-4)		6.99(-8)
	-2.43(-6)	
-1.07(-4)		1.08(-8)
	-6.01(-7)	
-3.80(-5)		1.71(-9)
	-1.49(-7)	
-1.35(-5)		2.74(-10)
	-3.70(-8)	
-4.81(-6)		

Table 5b. Example 3, $q = 1/2$.

-3.90(-2)		
	-1.85(-3)	
-1.75(-2)		8.05(-6)
	-4.56(-4)	
-7.61(-3)		5.63(-6)
	-1.10(-4)	
-3.26(-3)		1.55(-6)
	-2.63(-5)	
-1.39(-3)		3.50(-7)
	-6.31(-6)	
-5.87(-4)		7.35(-8)
	-1.52(-6)	
-2.48(-4)		1.50(-8)
	-3.69(-7)	
-1.04(-4)		3.04(-9)
	-9.01(-8)	
-4.39(-5)		

Table 5c. Example 3, $q = 3/4$.

Example 4: The final example is

$$(D^q(x-1))(t) + 4x(t) = 4e^t + \frac{t^{-q}}{\Gamma(1-q)}({}_1F_1(1; 1-q; t) - 4), \quad x(0) = 1,$$

with exact solution

$$x(t) = e^t.$$

In this example, we again observed convergence orders of n^{q-2} is the first, n^{-2} in the second, and n^{q-3} in the third column.

-9.13(-4)		
	-3.36(-5)	
-2.95(-4)		2.47(-7)
	-8.22(-6)	
-9.35(-5)		4.02(-8)
	-2.02(-6)	
-2.92(-5)		6.27(-9)
	-5.01(-7)	
-9.04(-6)		9.58(-10)
	-1.25(-7)	
-2.78(-6)		1.45(-10)
	-3.10(-8)	
-8.47(-7)		2.17(-11)
	-7.75(-9)	
-2.57(-7)		3.24(-12)
	-1.93(-9)	
-7.78(-8)		

Table 6a. Example 4, $q = 1/4$.

-1.80(-2)		
	-2.90(-4)	
-8.56(-3)		1.51(-6)
	-7.15(-5)	
-4.03(-3)		3.52(-7)
	-1.76(-5)	
-1.89(-3)		8.32(-8)
	-4.34(-6)	
-8.84(-4)		2.02(-8)
	-1.07(-6)	
-4.13(-4)		4.96(-9)
	-2.64(-7)	
-1.92(-4)		1.22(-9)
	-6.50(-8)	
-9.00(-5)		2.99(-10)
	-1.60(-8)	
-4.20(-5)		

Table 6b. Example 4, $q = 9/10$.

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