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MONOTONICITY RESULTS FOR A COMPOUND QUADRATURE METHOD FOR FINITE-PART INTEGRALS

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ABSTRACT. Given a function $f \in C^3[0,1]$ and some $q \in (0,1)$, we look at the approximation for the Hadamard finite-part integral $⨎_0^1 x^{-q-1} f(x)dx$ based on a piecewise linear interpolant for f at n equispaced nodes (i.e., the product trapezoidal rule). The main purpose of this paper is to give sufficient conditions for the sequence of approximations to converge against the correct value of the integral in a monotonic way. An application of the results yields detailed information on the error term of a backward differentiation formula for a fractional differential equation.

Key words and phrases: Hadamard finite-part integral; Quadrature formula; Product trapezoidal formula; Monotonicity; Fractional differential equation; Discrete Gronwall inequality; Backward differentiation formula.

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1. INTRODUCTION

When discussing problems in numerical integration, it is often not sufficient to prove that a certain sequence of approximations is convergent. Frequently one additionally wants to know whether the sequence converges in a monotonic fashion, i.e. whether one can be certain that an approximation using more quadrature nodes is actually better than an approximation with fewer nodes. Such monotonicity results are closely related to the question of finding so-called stopping rules: One needs to determine the value of an integral with a certain prescribed accuracy and the smallest possible amount of work.

For the classical setting when the integral in question is a standard unweighted integral $\int_a^b f(x)dx$, this topic is well investigated; we refer to the comprehensive survey of Förster [9] and the references cited therein and to the more recent papers [6, 10, 12] for a description of the present state of the art. However, to the best of our knowledge nothing is known about such

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results when the functional to be approximated is a weighted strongly singular integral of the form

$$I_q[f] := \fint_0^1 x^{-q-1} f(x)dx := \sum_{k=0}^{\lfloor q \rfloor} \frac{f^{(k)}(0)}{(k-q)k!} + \int_0^1 x^{-q-1} R_{\lfloor q \rfloor}(x)dx \tag{1.1}$$

interpreted in Hadamard's finite-part sense (see, e.g., [11] or [2, §1.6.1]). Here we assume q to be a positive non-integer number, and

$$R_\mu(x) := \frac{1}{\mu!} \int_0^x (x-y)^\mu f^{(\mu+1)}(y)dy$$

is the remainder of the Taylor polynomial of f, centered at 0. By $\lfloor q \rfloor$, we denote the largest integer not exceeding q. It is well known that a sufficient condition for the existence of $I_q[f]$ is that $f \in C^{\lfloor q \rfloor + 1}[0,1]$. Among the most important properties of these integral operators we mention here only that, in contrast to the classical Riemann or Lebesgue integral, I_q is not a positive functional, i. e. the inequality $|I_q[f]| \le I_q[|f|]$ is not true in general. Additional properties are described in [2, §1.6.1]. Since integrals of this type are known to have important applications in various methods for solving partial differential equations or ordinary differential equations of fractional (i.e., non-integer) order [3, 4, 7, 8, 11], we now aim to extend the classical theory to this setting.

Specifically we shall investigate what is probably the most important example of a quadrature formula for I_q, the product trapezoidal method. The construction of the method is simple: Given an integer n, we divide the fundamental integral $[0,1]$ into n subintervals of equal length with break points $x_j = \frac{j}{n}$, $j = 0, 1, \ldots, n$. We then replace the function f by its piecewise linear interpolant (linear interpolating spline) with knots and nodes at $x_0, x_1, \ldots, x_n$. Denoting this interpolant by f_{n+1} (the subscript $n+1$ being the number of interpolation points), we then define our approximation $I_{q,n+1}$ for I_q according to

$$I_{q,n+1}[f] := I_q[f_{n+1}],$$

where we note that the piecewise linear structure of f_{n+1} allows us to calculate the expression on the right-hand side effectively.

An explicit representation for $I_{q,n+1}$ is available from [3, Lemma 2.1]:

Lemma 1.1. *We have*

$$I_{q,n+1}[f] = \sum_{k=0}^{n} \alpha_{kn} f\left(\frac{k}{n}\right),$$

where

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

There are various reasons for choosing this formula as a first candidate for our investigations:

- It is a generalization of the classical trapezoidal formula, which is in turn the quadrature formula for standard integrals that was historically among the first and is very thoroughly investigated with respect to its monotonicity properties.
- Many other properties of this formula have been studied in great detail, see, e.g., [4, 5].
- It has been used very successfully as the basic ingredient for algorithms for the numerical solution of fractional differential equations [3].

2. MAIN RESULT

The main result of this paper is the following monotonicity theorem that directly corresponds to an analogous result for standard integrals (see, e.g., [13] or [1, Thm. 105]).

Theorem 2.1. *Let $0 < q < 1$ be fixed, and let $f \in C^3[0,1]$. Moreover assume that f'' is nonnegative on $[0,1]$ (i.e. f is convex) and f''' is nonpositive on $[0,1]$. Then, the sequence $(I_{q,n+1}[f])_{n=1}^{\infty}$ is monotonically decreasing, and its limit is $I_q[f]$.*

For the proof we shall use some properties of the quadrature rule $(I_{q,n+1})_{n=1}^{\infty}$ that have been established previously. Here and in the following we will make use of the notation

$$R_{n+1} := I_q - I_{q,n+1}$$

to denote the remainder functional of $I_{q,n+1}$. For the sake of simplicity we have suppressed the dependence on q in our notation. (Remember that q is assumed to be fixed.)

In view of the above mentioned properties of the functional I_q and its approximation $I_{q,n+1}$, we may apply the classical Peano kernel theorem [16] to R_{n+1} and derive

Lemma 2.2. *Let $0 < q < 1$ or $1 < q < 2$, and assume that $f \in C^2[0,1]$. Then,*

$$R_{n+1}[f] = \int_0^1 K_2(R_{n+1}, x) f''(x)dx,$$

where $K_2(R_{n+1}, \cdot)$ is the second Peano kernel of R_{n+1}, given by

$$K_2(R_{n+1}, x) := R_{n+1}[(\cdot - x)_+].$$

Here $(\cdot)_+$ is the truncated power function defined by

$$(x)_+ := \begin{cases} x & \text{if } x \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

From Lemma 2.2 we can deduce the explicit representation

$$K_2(R_{n+1}, t) = \sum_{k=0}^{j} \alpha_{kn} \left(\frac{k}{n} - t \right) - \frac{t^{1-q}}{q(1-q)} \quad \text{for } t \in \left[\frac{j}{n}, \frac{j+1}{n} \right] \tag{2.1}$$

of the Peano kernel in a straightforward way (as is done, e.g., in [1, Thm. 16] for classical quadrature formulas).

In [4, p. 487] it has been stated that R_{n+1} is negative definite of order two whenever $0 < q < 1$ or $1 < q < 2$. Unfortunately this result is incorrect; it should read as follows.

Lemma 2.3. *For any $n \geq 2$, the functional R_{n+1} is negative definite for $0 < q < 1$ and indefinite for $1 < q < 2$.*

Proof. It is clear that

$$\begin{aligned} R_{n+1}[f] &= I_q[f - f_{n+1}] \\ &= ⨍_0^{n^{-1}} u^{-q-1}(f(u) - f_{n+1}(u))du + \int_{n^{-1}}^1 u^{-q-1}(f(u) - f_{n+1}(u))du. \end{aligned}$$

To prove the negative definiteness in the case $0 < q < 1$ it is sufficient to show that $R_{n+1}[f] \leq 0$ whenever f is convex. Thus we assume f to be convex. Then, as is well known, $f(u) \leq f_{n+1}(u)$ for all u, and hence the second integral is nonpositive. Moreover, for the first integral we can explicitly calculate the Peano kernel representation

$$⨍_0^{n^{-1}} u^{-q-1}(f(u) - f_{n+1}(u))du =: A[f] = \int_0^{n^{-1}} f''(u) K_2(A, u)du.$$

In view of the relation between the functionals A and R_n, it is evident that for $u \in [0, n^{-1}]$ we have

$$K_2(A, u) = K_2(R_{n+1}, u) = -\frac{u}{q(1-q)}\left(u^{-q} - n^q\right) \le 0 \tag{2.2}$$

because of (2.1). Thus, the first integral is nonpositive too if f is convex, and the claim follows.

The indefiniteness in the case $1 < q < 2$ follows by very similar arguments. We find the same expression for the Peano kernel $K_2(A, \cdot)$ as above, but now the sign of $(1-q)$ and hence the sign of the complete expression has changed. Thus $K_2(A, u) \ge 0$ for $0 < u < n^{-1}$. Since nothing changes in the integral over $[n^{-1}, 1]$, we deduce that now R_{n+1} is the sum of a positive definite functional on $C^2[0, n^{-1}]$ and a negative definite functional on $C^2[n^{-1}, 1]$, and hence it must be indefinite. □

Formulated in terms of Peano kernels, the case $0 < q < 1$ of Lemma 2.3 can be restated as:

Lemma 2.4. *Let* $0 < q < 1$, $x \in [0, 1]$ *and* $n \in \mathbb{N}$. *Then,* $K_2(R_{n+1}, x) \le 0$.

Standard methods from elementary Peano kernel theory give us additional fundamental results on the function $K_2(R_{n+1}, \cdot)$ and its L_1 norm

$$\rho_{n+1} := \|K_2(R_{n+1}, \cdot)\|_1 = \int_0^1 |K_2(R_{n+1}, x)| dx;$$

we omit the details of the proof.

Lemma 2.5. *Let* $0 < q < 1$.

(a) *For* $j = 0, 1, \ldots, n$ *we have* $K_2(R_{n+1}, x_j) = 0$.
(b) *The sequence* $(\rho_{n+1})_{n=1}^{\infty}$ *is monotonically decreasing.*

Finally we quote another result on the sequence mentioned in Lemma 2.5 (b) from [5, Thm. 1.2]; more details are given there and in [4, Thm. 2.3].

Lemma 2.6. *For* $0 < q < 1$ *there exists some constant* c_q *such that* $\rho_{n+1} = c_q n^{q-2} + O(n^{-2})$.

We are now in a position to prove our main result.

Proof of Theorem 2.1. First we note that, by Lemmas 2.2 and 2.4,

$$R_{n+1}[f] = \int_0^1 K_2(R_{n+1}, x) f''(x) dx \le 0,$$

and hence by definition of R_{n+1} we find that $I_{q,n+1}[f] \ge I_q[f]$.

Moreover, by Lemma 2.2, Hölder's inequality and Lemma 2.6,

$$|R_{n+1}[f]| = \left| \int_0^1 K_2(R_{n+1}, x) f''(x) dx \right| \le \|f''\|_\infty \cdot \rho_{n+1} \to 0,$$

i.e. (again by definition of R_{n+1}), $I_{q,n+1}[f] \to I_q[f]$ as $n \to \infty$.

It remains to prove that the sequence $(I_{q,n+1}[f])$ decreases monotonically or, equivalently, that the sequence $(R_{n+1}[f])$ increases monotonically. To this end, we use the representation of $R_{n+1}[f]$ from Lemma 2.2 and introduce the functions J_{n+1} and L_{n+1} according to

$$J_{n+1}(x) := K_2(R_{n+1}, x) + \rho_{n+1} \qquad \text{and} \qquad L_{n+1}(x) := \int_0^x J_{n+1}(t) dt.$$

Then, a partial integration yields

$$\begin{aligned} R_{n+1}[f] &= \int_0^1 (J_{n+1}(x) - \rho_{n+1}) f''(x) dx \\ &= f''(x) \left[L_{n+1}(x) - x\rho_{n+1} \right]_0^1 - \int_0^1 f'''(x) \left[L_{n+1}(x) - x\rho_{n+1} \right] dx \\ &= f''(1) \left[L_{n+1}(1) - \rho_{n+1} \right] - \int_0^1 f'''(x) \left[L_{n+1}(x) - x\rho_{n+1} \right] dx \end{aligned}$$

since obviously $L_{n+1}(0) = 0$. Moreover,

$$\begin{aligned} L_{n+1}(1) &= \int_0^1 J_{n+1}(t) dt \\ &= \int_0^1 \left(K_2(R_{n+1}, x) + \rho_{n+1} \right) dx = \int_0^1 K_2(R_{n+1}, x) dx + \rho_{n+1}. \end{aligned}$$

Recalling the definition of ρ_{n+1} and the nonpositivity of $K_2(R_{n+1}, \cdot)$ (see Lemma 2.4), we find

$$\rho_{n+1} = \int_0^1 |K_2(R_{n+1}, x)| dx = -\int_0^1 K_2(R_{n+1}, x) dx,$$

and hence $L_{n+1}(1) = 0$ too. Combining these results we find

$$R_{n+1}[f] = -\rho_{n+1} f''(1) - \int_0^1 f'''(x) \left[L_{n+1}(x) - x\rho_{n+1} \right] dx.$$

Under our assumptions on f, we know that $f''(1) \geq 0$, and hence by Lemma 2.5 (b) we see that the first expression on the right-hand side, viz. the quantity $-\rho_{n+1} f''(1)$, is indeed a monotonically increasing function of n. It thus remains to prove that the remaining term has got this property as well. Since f''' is assumed to be negative, it is sufficient for this purpose to show that, for every fixed $x \in [0, 1]$, the function ϕ_x defined by

$$\phi_x(n + 1) := L_{n+1}(x) - x\rho_{n+1}$$

is a non-decreasing function of n. Note that

$$\phi_x(n + 1) = \int_0^x \left(K_2(R_{n+1}, t) + \rho_{n+1} \right) dt - x\rho_{n+1} = \int_0^x K_2(R_{n+1}, t) dt.$$

For the proof of the monotonicity of ϕ_x we distinguish two cases.

First we look at $0 \leq x \leq (n + 1)^{-1}$. An explicit representation for $K_2(R_{n+1}, t)$ in the case $0 < t < n^{-1}$ can be taken from eq. (2.1); it reads

$$K_2(R_{n+1}, t) = \frac{t}{q(1 - q)} \left(n^q - t^{-q} \right).$$

Consequently,

$$\phi_x(n + 1) = \frac{1}{q(1 - q)} \left(\frac{1}{2} n^q x^2 - \frac{1}{2 - q} x^{2-q} \right)$$

for $0 \leq x \leq n^{-1}$. In an analogous manner we find

$$\phi_x(n + 2) = \frac{1}{q(1 - q)} \left(\frac{1}{2} (n + 1)^q x^2 - \frac{1}{2 - q} x^{2-q} \right)$$

for $0 \leq x \leq (n + 1)^{-1}$. From these identities we immediately see

$$\phi_x(n + 1) \leq \phi_x(n + 2)$$

for all n and $0 \leq x \leq (n + 1)^{-1}$ as required.

In the second case $(n+1)^{-1} < x \le n^{-1}$ we will prove the relation

$$\phi_x(n+1) \le \phi_{(n+1)^{-1}}(n+1) \le \phi_{n^{-1}}(n+2) \le \phi_x(n+2).$$

Since $K_2(R_{n+1}, \cdot)$ is a nonpositive function (see Lemma 2.4), we find that $\phi_x(n+1)$ is a decreasing function of x. Thus the first and the last of the three inequalities above are evident. It remains to show the middle one. To this end we note that we still have, as above,

$$\phi_x(n+1) = \frac{1}{q(1-q)} \left(\frac{1}{2} n^q x^2 - \frac{1}{2-q} x^{2-q} \right),$$

and therefore

$$\begin{aligned} \phi_{(n+1)^{-1}}(n+1) &= \frac{1}{q(1-q)} \left(\frac{1}{2} n^q (n+1)^{-2} - \frac{1}{2-q} (n+1)^{q-2} \right) \\ &= \frac{1}{q(1-q)(n+1)^2} \left(\frac{1}{2} n^q - \frac{1}{2-q} (n+1)^q \right). \end{aligned}$$

However we now pass a node of the formula $I_{q,n+2}$, namely the point $(n+1)^{-1}$, and hence the Peano kernel K_2 of this formula becomes

$$\begin{aligned} K_2(R_{n+2}, t) &= -\alpha_{0,n+1} t + \alpha_{1,n+1} \left(\frac{1}{n+1} - t \right) - \frac{t^{1-q}}{q(1-q)} \\ &= \frac{(n+1)^q}{q(1-q)} \left(t + (2 - 2^{1-q}) \left(\frac{1}{n+1} - t \right) - (n+1)^{-q} t^{1-q} \right) \end{aligned}$$

according to eq. (2.1) and Lemma 1.1. Thus we have

$$\begin{aligned} \phi_{n^{-1}}(n+2) &= \int_0^{n^{-1}} K_2(R_{n+2}, t) dt \\ &= \int_0^{(n+1)^{-1}} K_2(R_{n+2}, t) dt + \int_{(n+1)^{-1}}^{n^{-1}} K_2(R_{n+2}, t) dt \\ &= \phi_{(n+1)^{-1}}(n+2) + \int_{(n+1)^{-1}}^{n^{-1}} K_2(R_{n+2}, t) dt \\ &= \frac{1}{q(1-q)} \left(\frac{1}{2} - \frac{1}{2-q} \right) (n+1)^{q-2} + \int_{(n+1)^{-1}}^{n^{-1}} K_2(R_{n+2}, t) dt \\ &= -\frac{1}{2(1-q)(2-q)} (n+1)^{q-2} + \int_{(n+1)^{-1}}^{n^{-1}} K_2(R_{n+2}, t) dt \\ &= -\frac{1}{2(1-q)(2-q)} (n+1)^{q-2} \\ &\quad + \frac{1}{2q(1-q)(2-q)} \big(2(n+1)^{q-2} - 2n^{q-2} \\ &\qquad\qquad + n^{-2}(n+1)^{q-2}(q-2)(1 - 2^{1-q} - 2n) \big), \end{aligned}$$

and after a rather long but simple calculation we obtain the required inequality.

On the remaining part of the interval $[0, 1]$, the required representation of the Peano kernel is also given in (2.1). For the purpose of illustration we have plotted the graphs for $\phi_x(n+1)$ versus x in Figure 2.1 for the special case $q = 0.3$ and $n \in \{5, 6, 7\}$. In a qualitative sense these graphs can be considered to be typical also for other values of $q \in (0, 1)$. Using these representations, we can deduce the required property after a lengthy but straightforward calculation on these intervals too. □

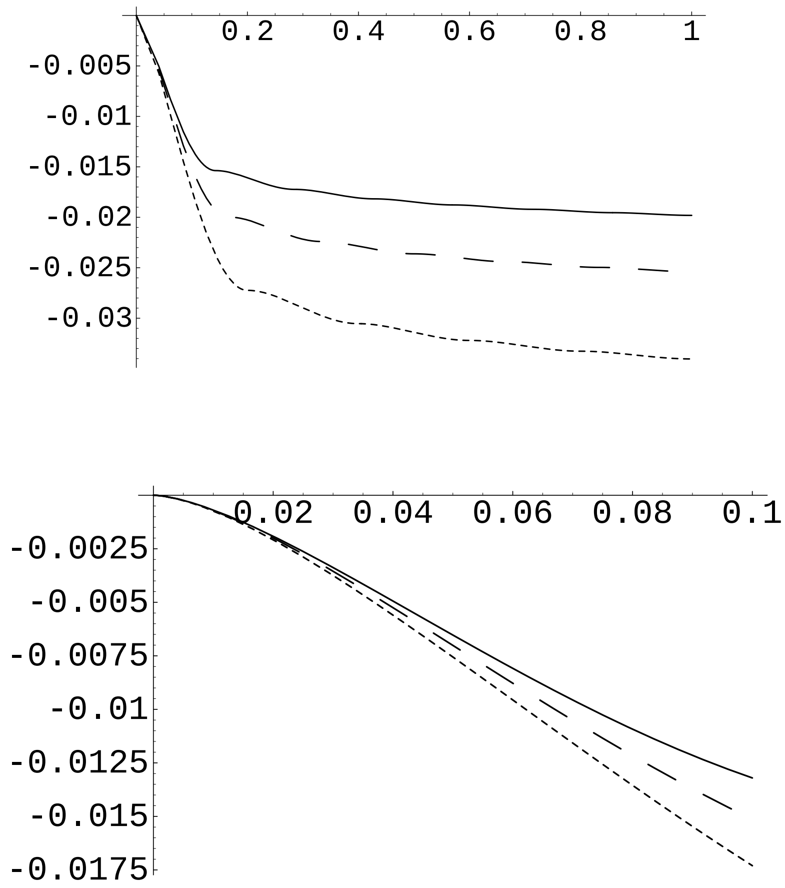

Figure 2.1: Plots of $\phi_x(n+1)$ versus x for $n = 5$ (dotted line; bottom), $n = 6$ (dashed line; middle), and $n = 7$ (solid line; top), over the entire interval $x \in [0, 1]$ (upper graph) and zoom over the subinterval $x \in [0, 0.1]$ (lower graph).

3. FURTHER REMARKS

In Lemma 2.3 we had pointed out a mistake in the discussion of the case $1 < q < 2$ in our earlier paper [4]. This observation leads to some consequences.

To begin with, an error estimate for the quadrature rule considered above has been discussed in [4, Thm. 2.3]. The analysis there was partly based on the incorrect result and needs to be modified slightly. The correction due to this problem affects only the case $1 < q < 2$ (the parameter p used in that paper corresponds to $q+1$ here), but since the original proof regrettably also contained some typographical errors in the case $0 < q < 1$, we give the correct result in both cases here.

Theorem 3.1. *Let $0 < q < 1$ or $1 < q < 2$. Then, for every $n \in \mathbb{N}$ we have*

$$\frac{30 - q(q+1)}{360q \cdot |1-q|(2-q)} n^{q-2} + \left(\frac{q+1}{180} - \frac{1}{6q}\right) n^{-2} < \rho_{n+1} < \left(\frac{1}{6q} + \frac{1}{2|1-q|(2-q)}\right) n^{q-2} - \frac{1}{6q} n^{-2}.$$

Proof. In [4, Proof of Thm. 2.3], we have seen that

$$\rho_{n+1} = \sigma + \tau,$$

where

$$\frac{1-n^{-q}}{q}\left(\frac{1}{6} - \frac{q(q+1)}{180}\right) n^{q-2} < \sigma < \frac{1-n^{-q}}{6q} n^{q-2}$$

and

$$\tau = \sup_{\|f''\|_\infty \le 1} |A[f]|,$$

where $A[f]$ is as in the proof of Lemma 2.3. Thus, standard Peano kernel theory reveals that

$$\tau = \int_0^{n^{-1}} |K_2(A,u)| du.$$

From the explicit representation of $K_2(A,\cdot)$ in eq. (2.2) we find that

$$\tau = \frac{1}{q\cdot|1-q|}\int_0^{n^{-1}} u(u^{-q} - n^q) du = \frac{n^{q-2}}{2|1-q|(2-q)},$$

and the claim follows. □

Another aspect of the results presented in §2 is related to the fact that finite-part integrals are a convenient means to represent derivatives of fractional order. To be precise, as is well known [7], we have that the Caputo-type fractional differential operator D_*^q can be rewritten as

$$D_*^q y(x) = \frac{1}{\Gamma(-q)} \,⨎_0^x (y(u) - y(0))(x-u)^{-q-1} du$$

for $0 < q < 1$ and as

$$D_*^q y(x) = \frac{1}{\Gamma(-q)} \,⨎_0^x (y(u) - y(0) - uy'(0))(x-u)^{-q-1} du$$

for $1 < q < 2$. We refer to the books of Podlubny [14] or Samko et al. [15] for detailed information on fractional derivatives and fractional differential equations; here we only note that our results above can be applied in a direct way to derive monotonically convergent approximations for such derivatives. We recall that certain other important properties of the approximation method investigated here have been given in [5].

Differential equations involving such operators have proven to be an important tool in many applications in physics, engineering, finance, etc.; see, e.g., the examples mentioned in [14] and the references cited therein. It is an obvious consequence of the above considerations that we may also use the product trapezoidal method for finite-part integrals as a means to construct numerical solutions for fractional differential equations. First results on this topic have been given in [3, 5]. In the analysis of the algorithm, a discrete Gronwall inequality [3, Lemma 2.3] turned out to be helpful. In view of our new developments above we may now strengthen this result and bring it into the form of a two-sided inequality:

Theorem 3.2. *For $0 < q < 1$, let the sequence (d_j) be given by $d_1 = 1$ and*

$$d_j = 1 + q(1-q)j^{-q} \sum_{k=1}^{j-1} \alpha_{kj} d_{j-k}, \qquad j = 2, 3, \ldots,$$

where α_{kj} is as in Lemma 1.1. Then,

$$j^q \le d_j \le \frac{\sin \pi q}{\pi q(1-q)} j^q, \qquad j = 1, 2, 3, \ldots.$$

We can thus see that the upper bound gives the correct rate of growth of the sequence (d_j).

Proof. The upper bound is known [3, Lemma 2.3]. For the lower bound, we proceed inductively. The induction basis ($j = 1$) is presupposed. For the induction step we use the fact that $\alpha_{kj} > 0$ for all j and k under consideration and find, using the function $\phi(x) = (1-x)^q$, that

$$\begin{aligned} d_{j+1} &= 1 + q(1-q)(j+1)^{-q} \sum_{k=1}^{j} \alpha_{k,j+1} d_{j+1-k} \\ &\geq 1 + q(1-q) \sum_{k=1}^{j+1} \alpha_{k,j+1} \left(\frac{j+1-k}{j+1} \right)^q \\ &= 1 + q(1-q) \left(I_{q,j+2}[\phi] - \alpha_{0,j+1}\phi(0) \right) \\ &= 1 + q(1-q) I_{q,j+2}[\phi] + (j+1)^q. \end{aligned}$$

It thus remains to prove that $q(1-q)I_{q,j+2}[\phi] \geq -1$. In view of the fact that $\phi''(x) < 0$ and $\phi'''(x) \geq 0$ for $0 < x < 1$, Theorem 2.1 allows us to conclude that it is sufficient for this purpose to show that $q(1-q)I_{q,2}[\phi] \geq -1$. An explicit calculation reveals that indeed

$$q(1-q)I_{q,2}[\phi] = q(1-q) \left(\alpha_{02} + \alpha_{12} 2^{-q} \right) = -2^q + 2 - 2^{1-q} \geq -1.$$

This completes the proof. □

It is our belief that the new lower bound may be useful in gaining an even better understanding of the properties of the differential equation solver; in particular we hope to prove that the error bound derived in [3, Thm. 1.1] is not improvable. But this will be the topic of a different paper.

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