Three algorithms for Hadamard finite-part integrals and fractional derivatives

David Elliott

Mathematics Department, University of Tasmania, GPO Box 252C, Hobart, Tasmania, 7001 Australia

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Abstract

Three algorithms for the evaluation of the Hadamard finite-part integral of the form \( \int_1^{\infty} \frac{f(t)}{(1 - t)^{1+\alpha}} \, dt \), where \( \alpha \) is a positive non-integer, are described. One algorithm is based on a knowledge of the Chebyshev series expansion of \( f \) on \( [-1, 1] \), the other two on polynomial interpolations to \( f \) at the zeros of \( T_n \), the Chebyshev polynomial of the first kind. Convergence theorems are given for each algorithm, and each algorithm is demonstrated numerically.

Keywords: Hadamard finite-part integral; Fractional derivative; Polynomial interpolation; Chebyshev polynomial; Convergence; Stability

1. Introduction

We shall be concerned with approximate methods for the evaluation of

\[
K^\alpha f := \frac{1}{\Gamma(-\alpha)} \int_{-1}^{1} f(y) \frac{y}{(1 - y)^{1+\alpha}},
\]

where \( \alpha \) is positive, not an integer, and such that

\[
n < \alpha < n + 1,
\]

for some \( n \in \mathbb{N}_0 \), where \( \mathbb{N}_0 = \{0, 1, 2, 3, \ldots \} \). The integral is to be interpreted as the Hadamard finite-part. Basic properties of \( K^\alpha f \) have been discussed in Elliott [5] and if we assume that \( f^{(n+1)} \in C[-1,1] \) then from Eq. (2.2) of [5] we have

\[
K^\alpha f = \sum_{k=0}^{n} \frac{f^{(k)}(-1)}{\Gamma(k + 1 - \alpha)} 2^{2-k} + \frac{1}{\Gamma(n + 1 - \alpha)} \int_{-1}^{1} (1 - y)^{n-\alpha} f^{(n+1)}(y) \, dy.
\]

1. e-mail: elliott@hilbert.maths.utas.edu.au.
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As a consequence of (1.2) and the continuity of \( f^{(n+1)} \) we see that the integral in (1.3) is, at worst, improper. We have also observed in [5, Theorem 2.1] that \( Kf \) is the fractional derivative of order \( \alpha \) of the function \( f \) defined on \([-1,1]\), at the point 1. The reader might like to refer to Oldham and Spanier [14] for further details.

Two algorithms for the approximate evaluation of \( Kf \), based on the use of Bernstein polynomials to approximate \( f \), have been described in [5]. These algorithms contrasted with those previously described in [10, 15] which were based on polynomial interpolation to \( f \) on \([-1,1]\). Kutt used equally spaced nodes whereas Paget chose his nodes to be the zeros of Legendre polynomials. We shall see in Section 6 the reason for Paget’s choice.

In Sections 2 and 3 we shall introduce two quadrature rules for the approximate evaluation of \( Kf \). In the first, we approximate \( f \) by the partial sums of its Chebyshev series expansion. In the second, we approximate \( f \) by the Lagrange interpolation polynomial based on the zeros of \( T_n \), the Chebyshev polynomial of the first kind of degree \( N \). Not unexpectedly, these two rules are closely connected.

Sufficient conditions for the convergence of these two rules are given in Section 4. The analysis of the second rule suggests a third algorithm which might be worth considering under certain conditions.

Some numerical examples of the rules are given in Section 5 where the problem of numerical instability is illustrated. The final section, Section 6, sums up the paper and indicates areas for further work.

2. Derivation of the first quadrature rule

For \( k \in \mathbb{N}_0 \), let \( T_k \) denote the Chebyshev polynomial of the first kind of degree \( k \); that is,

\[
T_k(x) := \cos k\theta \quad \text{where} \quad x = \cos \theta,
\]

\( \theta \in [0, \pi] \). The Chebyshev coefficient \( a_k \) of a function \( f \) given on \([-1,1]\) is defined by

\[
a_k := (2/\pi) \int_{-1}^{1} (1 - x^2)^{-1/2} f(x) T_k(x) \, dx,
\]

\( k \in \mathbb{N}_0 \). The \( N \)th partial sum \( s_N \) is defined by

\[
s_N(x) := \sum_{k=0}^{N-1} a_k T_k(x),
\]

where \( \sum' \) denotes a sum whose first term is halved. Obviously \( s_N \) will be a polynomial of degree \( \leq (N - 1) \).

To obtain our first quadrature rule \( Q_N^{(1)}f \) we shall simply approximate \( Kf \) by \( Ks_N \) so that

\[
Q_N^{(1)}f := Ks_N = \sum_{k=0}^{N-1} a_k K_t T_k.
\]
We need to consider $K^aT_k$. From [1, Eq. (22.5.47)] we have

$$T_k(x) = \sum_{j=0}^{k} \frac{(-k)_j(k)_j}{j!} \left( \frac{1-x}{2} \right)^j. \quad (2.5)$$

Here $(a)_j$ denotes the Pochhammer symbol

$$(a)_j = a(a + 1) \cdots (a + j - 1) = \Gamma(a + j)/\Gamma(a), \quad (2.6)$$

provided that the gamma function formulation is defined. From (2.6) and [5, Eq. (1.3)] we find that

$$K^a(1-x)j = \frac{(-x)_j}{\Gamma(1-x)(1-x)_j 2^a-j}. \quad (2.7)$$

Substituting (2.7) into (2.5) gives

$$K^aT_k = \frac{1}{2^a \Gamma(1-x)} \sum_{j=0}^{k} \frac{(-k)_j(k)_j(-x)_j}{(\frac{1}{2})_j(1-x)_j j!} = \frac{1}{2^a \Gamma(1-x)} \quad _3F_2 \left[ \begin{array}{c} -k, k, -x; 1 \\ \frac{1}{2}, 1-x \end{array} \right]. \quad (2.8)$$

see, for example, [7, Ch. IV]. Unfortunately the generalised hypergeometric function in (2.8) is not Saalschützian so that we cannot represent its value at 1 in a simple way. However, [16] has shown that if we write

$$g_k = _3F_2 \left[ \begin{array}{c} -k, k, -x; 1 \\ \frac{1}{2}, 1-x \end{array} \right], \quad (2.9)$$

then $g_k$ satisfies the three-term recurrence relation

$$(k + 1 - x)g_{k+1} - 2(1+x)g_k - (k - 1 + x)g_{k-1} = 0. \quad (2.10)$$

with $g_0 = 1$ and $g_1 = (1+x)/(1-x)$. From the asymptotic form for $k \gg 1$ given in [16, Eq. (11)] one finds that

$$g_k = \frac{2^{2x-1}}{\Gamma(2x) \sin(\pi x)} k^{2x} \left[ 1 + O(1/k^2) \right] + \frac{(-1)^x \pi}{2} \frac{1}{k^2} \left[ 1 + O(1/k^2) \right]. \quad (2.11)$$

On recalling that $x$ is positive we see that the first term dominates so that $|g_k|$ will grow with $k$ and forward recurrence with (2.10) will be stable.

Returning to (2.4) we have that

$$Q^{(1)}_N f = \frac{1}{2^a \Gamma(1-x)} \sum_{k=0}^{N-1} a_k g_k. \quad (2.12)$$

This is the first of our quadrature rules and is readily applied if we know the Chebyshev coefficients $a_k$ of the function $f$. For many elementary functions and some higher transcendental functions these coefficients have been tabulated, see [2; 11, Ch. 17; 12]. However, in general this will not be the case and we need a rule which is more widely applicable.
Before doing so, however, it is worth observing that there is a problem of instability which can occur with all these rules and which may be serious. If \( f \) and \( g \) have Chebyshev coefficients \( a_k, b_k \) respectively for \( k = 0(1)(N - 1) \) then from (2.4)

\[
|Q_N^{(1)}f - Q_N^{(1)}g| = \left| \sum_{k=0}^{N-1} (b_k - a_k)K^*T_k \right|.
\]

Suppose \( g \) is an approximation to \( f \) which is such that there is a relative error \( \varepsilon > 0 \) in each coefficient \( a_k, k = 0(1)(N - 1) \); that is,

\[
|b_k - a_k| \leq \varepsilon |a_k|, \quad k = 0(1)(n - 1).
\]

Then (2.13) and (2.14) give

\[
|Q_N^{(1)}f - Q_N^{(1)}g| \leq \varepsilon |a_{N-1}| \left| \sum_{k=0}^{N-1} a_k/a_{N-1} \right| |K^*T_{N-1}|/|K^*T_N|,
\]

where we assume that \( a_{N-1} \neq 0 \). Assuming \( |a_k/a_{N-1}| \leq 1 \) for \( k = 0(1)(N - 1) \) and furthermore that \( |K^*T_k/K^*T_{N-1}| \leq 1, k = 0(1)(N - 1) \), which is not unreasonable in the light of (2.11), (2.15) implies that for some \( c > 0 \),

\[
|Q_N^{(1)}f - Q_N^{(1)}g| \leq ce^{2N}|a_{N-1}|.
\]

The behaviour of the right-hand side of (2.16) obviously depends on that of \( |a_{N-1}| \). From [4, 6] we have asymptotic estimates of \( a_N \) for \( N \gg 1 \). For many entire functions \( |a_N| \sim O(c^{-N}/N!) \), for some \( c > 0 \). If \( f \) has a pole then \( |a_N| \sim O(e^{-N}) \) for some \( c > 1 \) and if \( f \) has an algebraic singularity then \( |a_N| \sim O(1/\varepsilon^{N}\beta) \) for some \( c \) and \( \beta > 0 \). It is possible that the right-hand side of (2.16) could become "large" even though \( \varepsilon \) is "small", thereby introducing instability. We shall have more to say about this later.

3. The second quadrature rule

We now come to our second quadrature rule which is more widely applicable than the first and is based on approximating \( f \) by a Lagrange interpolation polynomial. Let \( L_{N-1}(f) \) denote the Lagrange interpolation polynomial of degree \( \leq (N - 1) \) which takes the values of \( f \) at the \( N \) zeros of \( T_N \) in \((-1, 1)\). If \( x_{j,N}, j = 1(1)N \), denote the zeros of \( T_N \) then

\[
x_{j,N} = \cos((j - \frac{1}{2})\pi/N), \quad j = 1(1)N,
\]

and we have

\[
L_{N-1}(f; x) = \sum_{j=1}^{N} f(x_{j,N}) \ell_{j,N}(x)
\]

where

\[
\ell_{j,N}(x) = T_N(x)/(T'_N(x_{j,N})(x - x_{j,N}))
\]
for \( j = 1(1)N \). (For properties of Chebyshev polynomials, see [18]). Now we can write, see [18, Eq. (1.130)],

\[
\ell_{j,N}(x) = \frac{2}{N} \sum_{k=0}^{N-1} T_k(x_j, N) T_k(x),
\]

so that

\[
L_{N-1}(f; x) = \frac{2}{N} \sum_{j=1}^{N} f(x_j, N) \sum_{k=0}^{N-1} T_k(x_j, N) T_k(x).
\]

Our second quadrature rule \( Q^{(2)}_N f \) will be defined by

\[
Q^{(2)}_N f := K^2 L_{N-1}(f),
\]

and from (2.8), (2.9) and (3.5) we find

\[
Q^{(2)}_N f = \sum_{j=1}^{N} \mu_{j,N} f(x_j, N),
\]

say, where the coefficients \( \mu_{j,N} \) are defined by

\[
\mu_{j,N} = 2^{1-a} \frac{1}{\Gamma(1-a)} \frac{1}{N} \sum_{k=0}^{N-1} g_k T_k(x_j, N),
\]

for \( j = 1(1)N \). We note, in passing, that \( Q^{(2)}_N f \) is also derivable from \( \psi^{(1)}_N f \) by replacing the coefficients \( a_k \), as defined in (2.2), with the approximations \( A_{k,N} \), say, which are obtained by approximating the integrals in (2.2) with Gauss–Chebyshev quadrature sums evaluated at the zeros of \( T_N \). We shall omit the details.

From Eq. (3.8), we see that the coefficients \( \mu_{j,N} \) are independent of the function \( f \) so that, given \( N \) and \( \alpha \), they can be computed once and for all. From the construction of \( Q^{(2)}_N f \) we see that it is exact whenever \( f \) is a polynomial of degree \( \leq N - 1 \) so that, in particular, when \( f = 1 \) we have

\[
\sum_{j=1}^{N} \mu_{j,N} = K^2 1 = 1/(2^a \Gamma(1-a)).
\]

Before proceeding with the application of these rules we shall, in the next section, give sufficient conditions under which \( Q^{(1)}_N f \) and \( Q^{(2)}_N f \) converge to \( K^2 f \) in the limit as \( N \to \infty \). The discussion of the convergence of \( Q^{(2)}_N f \) will suggest the investigation of a third quadrature rule \( Q^{(3)}_N f \) for which we shall also state sufficient conditions for convergence.

4. Convergence of the quadrature rules and a new rule

In Section 4.1 we shall give sufficient conditions to guarantee the convergence of \( Q^{(1)}_N f \) to \( K^2 f \). In Section 4.2 we shall consider convergence of \( Q^{(2)}_N f \) which in turn gives rise, in Section 4.3, to a third quadrature rule \( Q^{(3)}_N f \) and discussion of its convergence.
4.1. Convergence of $Q_N^{(1)}f$ to $K^xf$

Theorem 4.1. Suppose $f \in C[-1,1]$ is such that

(i) $\sum_{k=0}^{\infty} |a_k| < \infty$,
(ii) $K^xf$ exists, and
(iii) $\sum_{k=0}^{\infty} |a_k||K^xT_k| < \infty$.

Then $\lim_{N \to \infty} Q_N^{(1)}f = K^xf$.

Proof. From (i) it follows that $\sum_{k=0}^{\infty} a_k T_k(x)$ converges absolutely and uniformly to $f(x)$ on $[-1,1]$. Now $K^x$ is a linear functional defined on an appropriate subset of $C[-1,1]$. In particular, $K^xT_k$ exists for $k \in \mathbb{N}_0$. Recalling that $Q_N^{(1)}f = \sum_{k=0}^{N-1} a_k K^xT_k$ we have

$$|K^xf - Q_N^{(1)}f| = \left| \sum_{k=N}^{\infty} a_k K^xT_k \right| \leq \sum_{k=N}^{\infty} |a_k| \cdot |K^xT_k|.$$ (4.1)

From (iii) we see that $\lim_{N \to \infty} |K^xf - Q_N^{(1)}f| = 0$. □

The problem with this theorem is twofold. Firstly, only in special cases do we know the coefficients $a_k$ explicitly. Secondly, we do not have an explicit expression for $K^xT_k$ in closed form. Consequently, we need a more readily applicable result, albeit a weaker one. To this end, let us recall the definition of the modulus of continuity $\omega$ of a continuous function. We have

$$\omega(f; \delta) := \sup_{|x-y| \leq \delta} |f(x) - f(y)|.$$ (4.2)

Next, we have the following upper bound for $|a_k|$.

Lemma 4.2. If, for some $q \in \mathbb{N}_0$, $f^{(q)} \in C[-1,1]$ then

$$|a_k| \leq ck^{-q} \omega(f^{(q)}; 1/k),$$ (4.3)

for $k \in \mathbb{N}$.

Proof. See [8]. □

We can now give a sufficient condition for convergence. Here $\mathbb{N}$ denotes the natural numbers $\{1, 2, 3, \ldots\}$.

Theorem 4.3. Suppose that, for some $q \in \mathbb{N}$, $f^{(q)}$ is Hölder continuous of index $\beta$, $0 < \beta \leq 1$, on $[-1,1]$. If $q > 2\alpha + 1 - \beta$, then

$$\lim_{N \to \infty} Q_N^{(1)}f = K^xf.$$ (4.4)
Proof. Since $f^{(q)}$ is Hölder continuous of index $\beta$ on $[-1, 1]$ then $\omega(f^{(q)}; 1/k) \leq c k^{-\beta}$. Consequently, from (4.1) and (4.3) we have

$$|K^z f - Q_N^{(1)} f| \leq \frac{c}{2^z |\Gamma(1 - q)|} \sum_{k = N}^{\infty} k^{-q - \beta} |g_k|.$$  \hspace{1cm} (4.5)

From (2.11) we have that for $k \gg 1$, $|g_k| \sim O(k^2)$. Consequently for $N \gg 1$

$$|K^z f - Q_N^{(1)} f| \leq c_1 \sum_{k = N}^{\infty} k^{2\alpha - q - \beta},$$  \hspace{1cm} (4.6)

for some constant $c_1$. The right-hand side tends to zero only if the series converges and convergence occurs provided $2\alpha - q - \beta < - 1$. The result follows at once. \hspace{1cm} \square

If we recall that $n < x < n + 1$, then requiring $q > 2\alpha + 1 - \beta$ will imply that we choose $q$ to be either $2n + 2$ or $2n + 3$. From (1.3) we assumed only that $f^{(n + 1)} \in C[-1, 1]$, so that the application of Theorem 4.3 requires a higher degree of smoothness for $f$ than was originally required. We shall return to this point in Section 4.3.

Finally, we might note that if the Chebyshev coefficients $a_k$ of $f$ converge rapidly enough then an asymptotic estimate of $|K^z f - Q_N^{(1)} f|$ for $N \gg 1$ may be given by the first term of the sum in (4.1); that is, $|a_N g_N / 2^z \Gamma(1 - x)|$. However, since $g_N$ is growing like $N^{2x}$, care must be taken with this estimate.

4.2. Convergence of $Q_N^{(2)} f$ to $K^z f$

Before stating our convergence theorem (see Theorem 4.6) we need two further results. In the first, we give an estimate for $\sum_{j = 1}^{N} |\mu_{j,N}|$ when $N$ is large. We shall use the notation that for $N \gg 1$, $a(N) \sim b(N)$ means that $\lim_{N \to \infty} a(N)/b(N) = 1$.

**Theorem 4.4.** For $N \gg 1$,

$$\sum_{j = 1}^{N} |\mu_{j,N}| \sim (2^x \Gamma(x)/(\pi \Gamma(2x))) N^{2x} \{\log N + c(x) + O(1/N^{\min(1,2x)})\}$$  \hspace{1cm} (4.7)

where

$$c(x) = \ln 2 - \psi(2x + 1) + \sum_{n = 1}^{\infty} \frac{2^{2n-1} - 1}{2^{4n-2}} B(2n, 1 + 2x) \zeta(2n),$$  \hspace{1cm} (4.8)

$\psi$ denoting the digamma function, $B$ the Beta function and $\zeta$ the Riemann zeta function.

**Proof.** From (3.8), on replacing $g_k$, for $k = 1(1)(N - 1)$, by the first term of (2.11) we obtain

$$\mu_{j,N} \sim \frac{2^x \Gamma(x) N^{2x}}{\Gamma(2x)} \left\{ \frac{1}{N} \sum_{k = 1}^{N} \left( \frac{k}{N} \right)^{2x} \cos[(j - \frac{1}{2})\pi k/N] + \frac{\Gamma(2x) \sin(\pi x)}{2^{2x} \pi N^{1 + 2x}} \right\}.$$  \hspace{1cm} (4.9)
For \( N \gg 1 \), the sum in (4.9) can be replaced by an integral to give
\[
\mu_{j,N} \sim \frac{2^s \Gamma(x) N^{2x}}{\Gamma(2x)} \int_0^1 x^{2x} \cos \left[ \left( j - \frac{1}{2} \right) \pi x \right] dx + O(1/N^{\min(1, 2x)}) + O(1/N^{1+2x}),
\]
(4.10)
since the integrand is Hölder continuous of index \( \min(1, 2x) \) on \([0, 1]\).
Integrating once by parts gives
\[
\int_0^1 x^{2x} \cos \left[ \left( j - \frac{1}{2} \right) \pi x \right] dx = \frac{(-1)^{j+1}}{(j - \frac{1}{2})!} \left\{ 1 + 2x(-1)^j \int_0^1 x^{2x-1} \sin \left[ \left( j - \frac{1}{2} \right) \pi x \right] dx \right\}.
\]
(4.11)
Now the second term in \{ \} on the right-hand side of (4.11) is always less than 1 in modulus so that (4.10) and (4.11) together give
\[
\text{sgn} \mu_{j, N} = (-1)^{j+1}, \quad j \in \mathbb{N} \text{ and } N \gg 1.
\]
(4.12)
As a consequence of this let us write
\[
S_N := \sum_{j=1}^N |\mu_{j,N}| = \sum_{j=1}^N (-1)^{j+1} \mu_{j,N}
\]
(4.13)
From (4.9) we have
\[
S_N \sim \frac{2^s \Gamma(x) N^{2x}}{\Gamma(2x)} \left\{ \frac{1}{N} \sum_{k=1}^N \left( \frac{k}{N} \right)^{2x} \sum_{j=1}^N (-1)^{j+1} \cos \left[ \left( j - \frac{1}{2} \right) k \pi / N \right] \right. \\
\left. + \frac{\Gamma(2x) \sin(\pi x)}{2^{2x} \pi N^{1+2x}} \sum_{j=1}^N (-1)^{j+1} \right\}.
\]
(4.14)
Now \( \sum_{j=1}^N (-1)^{j+1} = O(1) \) and it is readily verified that
\[
\sum_{j=1}^N (-1)^{j+1} \cos \left[ \left( j - \frac{1}{2} \right) \pi x \right] = \frac{(-1)^{N+1} \cos(N \pi x) + 1}{2 \cos \left( \frac{1}{2} \pi x \right)},
\]
(4.15)
for \( N \in \mathbb{N} \). From (4.14) and (4.15) we can write
\[
S_N \sim \frac{2^s \Gamma(x) N^{2x}}{\Gamma(2x)} \left\{ S_N^{(1)} + O(1/N^{1+2x}) \right\}
\]
(4.16)
where
\[
S_N^{(1)} := \frac{1}{N} \sum_{k=1}^N \left( \frac{k}{N} \right)^{2x} \frac{1 + (-1)^{N+k+1}}{2 \cos(\pi k / 2N)}.
\]
(4.17)
The definition of \( S_N^{(1)} \) can be rewritten as
\[
S_N^{(1)} = \frac{1}{N} \sum_{s=1}^{[N/2]} \left( \frac{N - 2s + 1}{N} \right)^{2x} \frac{1}{\sin \left[ (2s - 1) \pi / 2N \right]},
\]
(4.18)
where \([N/2]\) denotes the integer part of \((N/2)\).
Again, we may rewrite (4.18) as
\[
S_N^{(1)} = \frac{1}{N} \sum_{s=1}^{[N/2]} \left\{ \left( \frac{N - 2s + 1}{N} \right)^{2s} \frac{1}{\sin \left[ (2s - 1)\pi/2N \right]} - \frac{1}{\left( (2s - 1)\pi/2N \right)} \right\} + \frac{2}{\pi} \sum_{s=1}^{[N/2]} \frac{1}{2s - 1}.
\]
(4.19)

Now from [19, Eq. (0.132)],
\[
\frac{2}{\pi} \sum_{s=1}^{[N/2]} \frac{1}{2s - 1} = \frac{1}{\pi} \left( \ln [N/2] + \gamma + \ln 4 \right) + O\left( \frac{1}{N^2} \right),
\]
where \( \gamma \) is Euler's constant. Again, since for \( N \gg 1 \) we can replace the first summation in (4.19) by an integral we have
\[
S_N^{(1)} \sim \frac{1}{\pi} \{ \ln [N/2] + \gamma + \ln 4 \} + \frac{1}{2} \int_0^1 \left[ \frac{(1 - x)^{2x}}{\sin(\frac{1}{2}\pi x)} - \frac{1}{(\frac{1}{2}\pi x)} \right] dx + O\left( 1/N \min(1, 2\pi) \right).
\]
(4.20)

From [1, Eq. (4.3.68)] and [19, Eq. (7.516)] we find
\[
\frac{1}{\sin(\frac{1}{2}\pi x)} = \frac{1}{(\frac{1}{2}\pi x)} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\gamma(2n-1) - 1}{2^{4n-2}} \zeta(2n)x^{2n-1},
\]
(4.21)
where \( \zeta \) denotes the Riemann zeta function. From (4.20) and (4.21)
\[
S_N^{(1)} \sim \frac{1}{\pi} \left\{ \ln N + \ln 2 + \gamma + O\left( 1/N \min(1, 2\pi) \right) \right\} + \int_0^1 \frac{(1 - x)^{2x} - 1}{x} dx
\]
\[+ \sum_{n=1}^{\infty} \frac{\gamma(2n-1) - 1}{2^{4n-2}} \zeta(2n) \int_0^1 (1 - x)^{2x} x^{2n-1} dx \right\}.
\]

From [1, Eqs. (6.3.22) and (6.2.1)] Eqs. (4.7) and (4.8) follow. \(\square\)

The second result is one that is often referred to as Gopengauz' theorem. A recent paper by Kilgore [9] discusses it at some length and we shall state it in a form suitable for our application. But first we define, for all \( f \in C_{[-1, 1]} \),
\[
E_n(f) := \inf_{-1 \leq x \leq 1} \max_{-1 \leq x \leq 1} |f(x) - p_n(x)|,
\]
(4.22)
where the infimum is taken over all polynomials \( p_n \) of degree \( \leq n \).

**Theorem 4.5.** With \( n < x < n + 1 \), suppose that \( f^{(2n+2)} \in C[-1, 1] \). If \( N > 4n + 5 \) then there exists a polynomial \( G_{N-1} \) say, of degree \( \leq N - 1 \) such that for all \( x \in [-1, 1] \),
\[
|f^{(k)}(x) - G_{N-1}^{(k)}(x)| \leq c \left( \frac{(1 - x^2)^{1/2}}{(N - 1)} \right)^{2n+2-k} E_{N-2n-3}(f^{(2n+2)}),
\]
(4.23)
for \( k = 0(1)(2n + 2) \), where \( c \) is independent of \( N \).

**Proof.** See [9]. \(\square\)
We are now in a position to state and prove sufficient conditions for the convergence of $Q_N^{(2)}f$ to $K^xf$.

**Theorem 4.6.** Suppose $n < \alpha < n + 1$, where $n \in \mathbb{N}_0$, and that $f^{(2n+2)} \in C[-1,1]$. Then
\[ \lim_{N \to \infty} Q_N^{(2)}f = K^xf. \]

**Proof.** Recalling from (3.6) that $Q_N^{(2)}f = K^xf$ whenever $f$ is a polynomial of degree $\leq (N - 1)$, we have
\[ K^xf - Q_N^{(2)}f = K^x(f - G_{N-1}) - Q_N^{(2)}(f - G_{N-1}) \]
(4.24)
where, for $N > 4n + 5$, $G_{N-1}$ is the Gopengauz polynomial as defined in Theorem 4.5. From (1.3), since $f^{(k)}(-1) = G_{N-1}^{(k)}(-1)$ for $k = 0(1)n$, we have
\[ K^x(f - G_{N-1}) = \frac{1}{\Gamma(n + 1 - \alpha)} \int_{-1}^{1} (1 - y)^{n-\alpha} (f^{(n+1)}(y) - G_{N-1}^{(n+1)}(y)) \, dy. \]  
(4.25)
From (4.23) with $k = n + 1$ we have
\[ |K^x(f - G_{N-1})| \leq \frac{cE_{N-2n-3}(f^{(2n+2)})}{(N - 1)^{n+1} \Gamma(n + 1 - \alpha)} \int_{-1}^{1} (1 - y)^{n-\alpha}(1 - y^2)^{n+1/2} \, dy. \]  
(4.26)
Since the integral is independent of $N$ we have at once that $\lim_{N \to \infty} K^x(f - G_{N-1}) = 0$.

Consider now the second term on the right-hand side of (4.24). From (3.7) and (4.23) with $k = 0$ we have
\[ |Q_N^{(2)}(f - G_{N-1})| \leq \frac{cE_{N-2n-3}(f^{(2n+2)})}{(N - 1)^{n+2}} \sum_{j=1}^{N} |\mu_{j,N}|(1 - x_{j,N}^2)^{n+1}. \]  
(4.27)
From Theorem 4.4, we have for $N \gg 1$,
\[ \sum_{j=1}^{N} |\mu_{j,N}|(1 - x_{j,N}^2)^{n+1} \leq C \cdot N^{2\alpha} \log N, \]
where $C$ is independent of $N$. Consequently
\[ |Q_N^{(2)}(f - G_{N-1})| \leq cE_{N-2n-3}(f^{(2n+2)}) \log N / N^{2(n+1 - \alpha)}, \]  
(4.28)
for some constant $c$. Since $\alpha < n + 1$, see (1.2), we have at once that $\lim_{N \to \infty} |Q_N^{(2)}(f - G_{N-1})| = 0$ and the theorem follows.

The fact that $\sum_{j=1}^{N} |\mu_{j,N}| \sim O(N^{2\alpha} \log N)$ for $N \gg 1$ is a result for numerical concern. Suppose $f_1, f_2$ are two functions such that $\|f_1 - f_2\|_\infty < \varepsilon$. Then
\[ |Q_N^{(2)}f_2 - Q_N^{(2)}f_1| = |Q_N^{(2)}(f_2 - f_1)| \leq \varepsilon \cdot O(N^{2\alpha} \log N). \]
Since $\alpha > 0$ then as $N$ increases the right-hand side can become arbitrarily large so that again (recall Section 2) we have instability in the algorithm. We shall consider an example of this in Section 5.
4.3. The quadrature rule $Q^{(3)}_N f$

The conditions of Theorem 4.6 are a little unsatisfactory in that for convergence we assume that $f$ is smoother than it needs to be for $K^*f$ to exist. We can obtain a mathematically more pleasing result by using a polynomial approximation to $f$, again based on interpolation at the zeros of $T_N$ [13]. We shall not consider Muneer's approximation [13] in full detail but will simplify the analysis by assuming that $f$ is such that

$$f^{(k)}(-1) = f^{(k)}(1) = 0 \quad \text{for } k = 0(1)n. \quad (4.29)$$

In principle, one can always achieve this by subtracting from any $f \in C^{(n+1)}[-1, 1]$ an appropriate polynomial of degree $(2n + 1)$ but we shall not pursue the details here. With $f$ satisfying (4.29) we construct the polynomial $M_{N+2n+1}$ say, of degree $\leq N + 2n + 1$, defined by

$$M_{N+2n+1}(f; x) := \sum_{j=1}^{N} \frac{f(x_{j,N})}{(1 - x_{j,N}^2)^{n+1}} \frac{(1 - x^2)^{n+1} T_N(x)}{T_N(x_{j,N})(x - x_{j,N})}, \quad (4.30)$$

where $T_N(x_{j,N}) = 0$, $j = 1(1)N$; see [13, Eq. (1.18)].

We observe that

$$M^{(k)}_{N+2n+1}(f; -1) = M^{(k)}_{N+2n+1}(f; 1) = 0, \quad (4.31)$$

for $k = 0(1)n$.

**Theorem 4.7.** Let $f^{(n+1)} \in C[-1, 1]$ with $f^{(k)}(-1) = f^{(k)}(1) = 0$ for $k = 0(1)n$. Then for all $x \in [-1, 1]$

$$|f^{(k)}(x) - M^{(k)}_{N+2n+1}(f; x)| \leq cN^{-n-1+k} \omega(f^{(n+1)}; 1/(N + 2n + 1)) \log N, \quad (4.32)$$

for $k = 0(1)(n + 1)$.

**Proof.** See [13, Theorem 1.2]. \[\square\]

We shall now introduce our third quadrature rule $Q^{(3)}_N f$ which is defined by

$$Q^{(3)}_N f := K^*M_{N+2n+1}(f). \quad (4.33)$$

From (4.30) we have

$$K^*M_{N+2n+1}(f) = \sum_{j=1}^{N} \frac{f(x_{j,N})}{(1 - x_{j,N}^2)^{n+1}} K^*\{(1 - x^2)^{n+1} \ell_{j,N}(x)\}, \quad (4.34)$$

where $\ell_{j,N}$ is defined in (3.3). Now, from (1.1)

$$K^*\{(1 - x^2)^{n+1} \ell_{j,N}(x)\} = \frac{1}{\Gamma(-\alpha)} \int_{-1}^{1} (1 - y)^{\alpha} y^n (1 + y)^{n+1} \ell_{j,N}(y) dy, \quad (4.35)$$
the integral now being an improper integral. Recalling (3.4) we have

\[
K^x \{(1 - x^2)^{n+1} \ell_{j,N}(x)\} = \frac{2}{\Gamma(-\alpha)N} \sum_{k=0}^{N-1} T_k(x_{j,N}) \int_{-1}^{1} (1 - y)^{n-\alpha}(1 + y)^{n+1} T_k(y) \, dy. \tag{4.36}
\]

From [16] we shall write

\[
\int_{-1}^{1} (1 - y)^{n-\alpha}(1 + y)^{n+1} T_k(y) \, dy = 2^{2n+1-\alpha} \frac{\Gamma(n - \alpha + 1)\Gamma(n + 2)}{\Gamma(2n - \alpha + 3)} h_k \tag{4.37}
\]
say, where the numbers \(h_k\) satisfy the three-term recurrence relation

\[
(k + 2n - \alpha + 3)h_{k+1} - 2(1 + \alpha)h_k - (k - 2n + \alpha - 3)h_{k-1} = 0 \tag{4.38}
\]
with \(h_0 = 1, \ h_1 = (1 + \alpha)/(2n - \alpha + 3)\).

From (4.33)-(4.37) we have

\[
Q_N^{(3)} f = \sum_{j=1}^{N} v_{j,N} f(x_{j,N})/(1 - x_{j,N}^2)^{n+1} \tag{4.39}
\]
where the coefficients \(v_{j,N}\) are given by

\[
v_{j,N} = \frac{2^{2n+3-\alpha}\Gamma(n - \alpha + 1)\Gamma(n + 2)}{\Gamma(-\alpha)\Gamma(2n - \alpha + 3)} \frac{1}{N} \sum_{k=0}^{N-1} h_k T_k(x_{j,N}), \tag{4.40}
\]
for \(j = 1(1)N\).

We can now give a convergence theorem for \(Q_N^{(3)} f\).

**Theorem 4.8.** Suppose \(n < \alpha < n + 1\) where \(n \in \mathbb{N}_0\) and that \(f^{(n+1)}(1) \in C[-1,1]\) with \(f^{(k)}(-1) = f^{(k)}(1) = 0\) for \(k = 0(1)n\). If \(f^{(n+1)}\) satisfies the Dini-Lipschitz condition that \(\lim_{\delta \to 0^+} \omega(f^{(n+1)}; \delta) \log \delta = 0\) then \(\lim_{N \to \infty} Q_N^{(3)} f = K^x f\).

**Proof.** From (1.3), (4.31), (4.32) with \(k = n + 1\) and (4.33) we have simply that

\[
|K^x(f - M_{N+2n+1}(f))| = \left| \frac{1}{\Gamma(n + 1 - \alpha)} \int_{-1}^{1} (1 - y)^{n-\alpha}(f^{(n+1)}(y) - M_{N+2n+1}^{(n+1)}(f; y)) \, dy \right| \leq c \omega(f^{(n+1)}; 1/(N + 2n + 1)) \log N, \tag{4.41}
\]
for some constant \(c\) independent of \(N\). Convergence now follows at once since \(f^{(n+1)}\) is assumed to satisfy the Dini-Lipschitz condition. \(\square\)

This convergence can be considered as mathematically satisfactory in the sense that we do not require \(f\) to possess a continuous derivative of higher order than that assumed for \(K^x f\) to exist.

It should be noted that in fact what we have produced here is a quadrature rule for the evaluation of the improper integral

\[
\frac{1}{\Gamma(n + 1 - \alpha)} \int_{-1}^{1} (1 - y)^{n-\alpha} f^{(n+1)}(y) \, dy
\]
since we see from (1.3) that the summation is zero. We note that $Q_N^{(3)} f$ is a quadrature sum involving the values of $f$ at the zeros of $T_N$ and does not involve any of the derivatives of $f$. We do not propose to consider the stability of this rule in this paper.

5. Some numerical examples

Let us apply $Q_N^{(1)}$ to the function $\exp(x)$. From [14, Section 6.2] we have that

$$K^x \exp(x) = \frac{1}{\Gamma(1 - \alpha)} \{e^{-1}2^{-x} + e \cdot \gamma(1 - \alpha, 2)\},$$

(5.1)

where $\gamma$ denotes the incomplete gamma function. In particular we find

$$K^{1/2} \exp(x) = e^{-1}(2\pi)^{-1/2} + e \cdot \text{erf}(\sqrt{2}) = 2.74136195,$$

(5.2)

$$K^{3/2} \exp(x) = K^{1/2} \exp(x) - 1/(4e(2\pi)^{1/2}) = 2.70467128.$$

In Table 1 we list the error $e_{N,\alpha}^{(1)}$ where

$$e_{N,\alpha}^{(1)}(f) := |K^x f - Q_N^{(1)} f|$$

(5.3)

for $\alpha = 0.5, 1.5$ and $N = 4(1)8$. The values of the Chebyshev coefficients of $\exp(x)$ are given in [2]. Additionally in Table 1 we have also noted the asymptotic value of the first neglected term $|a_N g_N/(2^x \Gamma(1 - \alpha))|$ which from (2.11) is given by

$$d_{N,\alpha}(f) = \sqrt{\pi} N^{2\alpha} |a_N|/(2^\alpha \Gamma(\alpha + \frac{1}{2})).$$

(5.4)

We see that in each case, even for the modest values of $N$ given, the sum $Q_N^{(1)} f$ is converging rapidly to $K^x f$. The values of the estimates $d_{N,\alpha}$ have been given to 3 significant digits in each case and we see that these estimates are reasonable although they underestimate the actual values. It should be noted, however, that the Chebyshev coefficients $a_k$ of the function $\exp(x)$ converge like $1/2^{k-1} k!$, which is rapid. Again since we have chosen only modest values of $\alpha$, this contributes to the reasonableness of the error estimates; this will not always be the case.

<table>
<thead>
<tr>
<th>$\alpha$ = 0.5</th>
<th>$\alpha$ = 1.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$e_{N,0.5}^{(1)}(f)$</td>
</tr>
<tr>
<td>4</td>
<td>0.03124435</td>
</tr>
<tr>
<td>5</td>
<td>0.00376874</td>
</tr>
<tr>
<td>6</td>
<td>0.00036853</td>
</tr>
<tr>
<td>7</td>
<td>0.0*3013</td>
</tr>
<tr>
<td>8</td>
<td>0.0*0207</td>
</tr>
</tbody>
</table>
In Table 2 we apply the quadrature rule $Q^{(2)}_N f$ to the exponential function, using the same values of $\alpha$ as in Table 1. We define

$$e^{(2)}_{N,\alpha}(f) := |K^\alpha f - Q^{(2)}_N f|.$$

(5.5)

In comparing common entries in Tables 1 and 2 we see that $e^{(2)}_{N,\alpha}(f)$, not surprisingly, is always larger than $e^{(1)}_{N,\alpha}(f)$ but not greatly so.

We consider again the use of the quadrature rule $Q^{(2)}_N f$, this time to the function $f(x) = (1 + x)^c$ where $c > 0$ and not an integer. On writing

$$(1 + x)^c = 2^c \left(1 - \frac{1 - x}{2}\right)^c = 2^c \sum_{j=0}^{\infty} \frac{(-c)_j}{j!} \left(\frac{1 - x}{2}\right)^j,$$

using (2.7) and [1, Eqs. (15.1.1) and (15.1.20)] we obtain

$$K^\alpha (1 + x)^c = 2^{-\alpha} \frac{\Gamma(c + 1)}{\Gamma(c + 1 - \alpha)}.$$ (5.6)

In Table 3 we have tabulated $e^{(2)}_{N,\alpha} f$ in two cases.

It should be noted that

$$K^{1.25} (1 + x)^{1.1} = 0.84778395, \quad K^{0.9} (1 + x)^{2.1} = 4.58231456.$$ (5.7)

Consider the case $\alpha = 1.25$, $c = 1.1$. The error appears to be converging to zero and if we assume that it is of the form $cN^{-r},$ for some constants $c$ and $r,$ then we find that $r = 1.7,$ approximately. For the function $(1 + x)^c,$ its Chebyshev coefficient $a_N$ is $O(1/N^{1 + 2c})$ see, for example, [4], so that from (5.4) we have that $d_{N,\alpha}(f) = O(1/N^{1 + 2c - 2\alpha}).$ This gives $d_{N,\alpha}(f) = O(1/N^{0.7})$ which is a pessimistic estimate of the observed rate of convergence. A similar comment can be made of the second case where $\alpha = 0.9$, $c = 2.1$. Here the errors appear to be converging to zero like $1/N^{4.4}$, whereas $d_{N,\alpha}(f) = O(1/N^{3.4})$ in this case. One further comment on Table 3 should be made. Although the case $\alpha = 1.25$, $c = 1.1$ exhibits convergence, the conditions of Theorem 4.6 are not satisfied. The conditions of that theorem are satisfied in the second case where $\alpha = 0.9$, $c = 2.1$.

We have illustrated the effects of instability in Table 4. Here we have chosen $f$ to be $(1 - x)^c$ so that an elementary calculation gives

$$K^\alpha (1 - x)^c = \frac{-2^{c-\alpha} \Gamma(1 + x) \sin(\pi x)}{\pi(c - x)}.$$ (5.8)

<table>
<thead>
<tr>
<th>Table 2</th>
<th>The function exp(x)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$e^{(2)}_{N,0.5}(f)$</td>
</tr>
<tr>
<td>5</td>
<td>0.00400700</td>
</tr>
<tr>
<td>7</td>
<td>0.043175</td>
</tr>
<tr>
<td>9</td>
<td>0.040014</td>
</tr>
<tr>
<td>11</td>
<td>0 to 8D</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3</th>
<th>$e^{(2)}_{N,\alpha} f$ for the function $f(x) = (1 + x)^c$ for $\alpha = 1.25$, $c = 1.1$ and $\alpha = 0.9$, $c = 2.1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$e^{(2)}_{N,\alpha}(f)$</td>
</tr>
<tr>
<td>10</td>
<td>0.00566394</td>
</tr>
<tr>
<td>20</td>
<td>0.00175296</td>
</tr>
<tr>
<td>40</td>
<td>0.00054036</td>
</tr>
<tr>
<td>80</td>
<td>0.00016638</td>
</tr>
<tr>
<td>160</td>
<td>0.045122</td>
</tr>
</tbody>
</table>
Table 4
The function \((1 - x)^c\) for 
\(x = 5.0001, c = 12.1\)

<table>
<thead>
<tr>
<th>N</th>
<th>(e^{(2)}_{N,x}(f))</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>0.0766</td>
</tr>
<tr>
<td>19</td>
<td>0.0342</td>
</tr>
<tr>
<td>20</td>
<td>0.0227</td>
</tr>
<tr>
<td>21</td>
<td>0.0263</td>
</tr>
<tr>
<td>22</td>
<td>0.0263</td>
</tr>
<tr>
<td>30</td>
<td>0.2290</td>
</tr>
<tr>
<td>40</td>
<td>61.3806</td>
</tr>
</tbody>
</table>

Table 5
\(e^{(3)}_{N,x}f\) for \(f(x) = (1 - x)^c(1 + x)^d\) for
\(x = 0.9, c = 1.3\) and \(d = 1.8\)

<table>
<thead>
<tr>
<th>N</th>
<th>(e^{(3)}_{N,x}(f))</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>0.10686094</td>
</tr>
<tr>
<td>80</td>
<td>0.06136116</td>
</tr>
<tr>
<td>160</td>
<td>0.03524070</td>
</tr>
<tr>
<td>320</td>
<td>0.02024018</td>
</tr>
<tr>
<td>640</td>
<td>0.01162489</td>
</tr>
<tr>
<td>1280</td>
<td>0.00667674</td>
</tr>
</tbody>
</table>

On choosing \(x = 5.0001\) and \(c = 12.1\) we have that \(K^x(1 - x)^c = 0.231894\). With these values of \(x\) and \(c\) the conditions of Theorem 4.6 are satisfied so that we expect convergence of \(Q^{(2)}_N f\) to \(K^x f\) in this case. In Table 4 we have tabulated \(e^{(2)}_{N,x,f}\), see (5.5), against \(N\).

As can be seen the error is a minimum when \(N = 20\) (being of the order of 10% of the required value) and then increases as \(N\) increases. By the time \(N = 40\) we see that the error is about 260 times the required value. This occurrence of instability when \(x\) is "large" is well known for the evaluation of these integrals and has been reported in [10, 15] and more recently in [17] who have suggested a resolution of the problem for their particular set of quadrature rules.

We conclude this section by one illustration of the rule \(Q^{(3)}_N f\) in the case when \(f(x) = (1 - x)^c(1 + x)^d\), for which we have, on using (5.6),

\[
K^x f = \frac{2^{c+d-x} \Gamma(d+1) \Gamma(c-x)}{\Gamma(-x) \Gamma(c+d-x+1)}. \tag{5.9}
\]

In Table 5 we display

\[
e^{(3)}_{N,x,f} := |K^x f - Q^{(3)}_N f| \tag{5.10}
\]

for a particular choice of \(x\), \(c\) and \(d\).

From Table 5, it appears that the quadrature rule is converging, albeit rather slowly, like \(O(1/N^{0.8})\). From (4.41), since \(n = 0\) in this case, we see that an upper bound for the error is \(O(\log N/N^{\min(c,d)-1})\) or \(O(\log N/N^{0.3})\) which is conservative.

6. Conclusion

Of the three algorithms described in this paper, \(Q^{(2)}_N f\) is the most versatile although problems can arise because of the inherent instability when \(x\) is "large". It is of interest to compare \(Q^{(2)}_N f\), based on interpolation at the zeros of \(T_N\), with the algorithm described in [15] who interpolated at the zeros of the Legendre polynomial \(P_N\). Paget's reason for choosing \(P_N\) has now become clearer. On repeating the analysis of Eqs. (2.5)-(2.8) with \(P_N\) instead of \(T_N\), one finds that the resulting \(_3F_2\) function is Saalschützian (see [7, Section 4.4]) so that it is readily summable in terms of gamma
functions. The evaluation of $K^a P_N$ essentially involves a two-term recurrence relation in place of the three-term recurrence relation of (2.10). It is doubtful whether this simplification justifies the work needed to compute the zeros of $P_N$ and the corresponding Christoffel numbers.

The problem of instability which is forever present with the evaluation of Hadamard finite-part integrals needs further attention. In [5] we have defined the condition number $\kappa_N$ of a quadrature rule of the form $\sum_{j=1}^{N} \mu_j N f(x_j, N)$ as
\begin{equation}
\kappa_N := \left| \sum_{j=1}^{N} \mu_j \right| / \sum_{j=1}^{N} \mu_j. \tag{6.1}
\end{equation}
Thus for Gaussian quadrature one has $\kappa_N = 1$ for all $N \in \mathbb{N}$. From (3.9) and (4.7) we see that for the quadrature rule $Q_N^{(2)} f$ we have
\begin{equation}
\kappa_N = \frac{2^{2a}}{\Gamma(2a)\sin(\pi a)} N^{2a} \log N \tag{6.2}
\end{equation}
for $N \gg 1$. On the other hand for the rules described in [5] based on the Bernstein polynomials we find
\begin{equation}
\kappa_N = A(\alpha) N^a \tag{6.3}
\end{equation}
for $N \gg 1$ where
\begin{equation}
A(\alpha) = \begin{cases} 
(-2a) \sum_{j=0}^{n/2} \frac{\Gamma(2j - \alpha)}{\Gamma(2j + 1)}, & n \text{ even,} \\
(-2a) \sum_{j=0}^{(n+1)/2} \frac{\Gamma(2j - 1 - \alpha)}{\Gamma(2j - 1)}, & n \text{ odd.} 
\end{cases} \tag{6.4}
\end{equation}
Thus we see that the rule based on Bernstein polynomials has better stability properties than that based on the zeros of $T_N$.

Although we have given proofs of convergence, more work needs to be done on realistic estimates of rates of convergence. The use of $|a_N K^a T_N|$ as an estimate for $|K^a f - Q_N^{(2)} f|$ is not satisfactory.

Other Hadamard finite-part integrals such as
\begin{equation}
\frac{1}{\Gamma(-\alpha)} \int_{-1}^{1} \frac{f(y) dy}{(1 + y)^{1+a}} \quad \text{and} \quad \frac{1}{\Gamma(-\alpha)} \int_{-1}^{1} \frac{f(y) dy}{|y - x|^{1+a}}, \quad x \in (-1, 1)
\end{equation}
are also of considerable importance and can be evaluated using the techniques of this paper by applying appropriate linear transformation on the variable of integration. These transformations have been discussed in detail in [3] and will not be considered here.

Acknowledgements

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like to thank the referee for his constructive comments which have greatly improved the presentation.

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