Numerical differentiation inspired by a formula of R.P. Boas

Gerhard Schmeisser

Department of Mathematics, University of Erlangen-Nuremberg, 91054 Erlangen, Germany

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Abstract

First, we briefly discuss three classes of numerical differentiation formulae, namely finite difference methods, the method of contour integration, and sampling methods. Then we turn to an interpolation formula of R.P. Boas for the first derivative of an entire function of exponential type bounded on the real line. This formula may be classified as a sampling method. We improve it in two ways by incorporating a Gaussian multiplier for speeding up convergence and by extending it to higher derivatives. For derivatives of order σ, we arrive at a differentiation formula with N′ nodes that applies to all entire functions of exponential type without any additional restriction on their growth on the real line. It has an error bound that converges to zero like e−3N/Nm as N → ∞, where α > 0 and N′ = 2N, m = 3/2 for odd σ while N′ = 2N + 1, m = 5/2 for even σ. Comparable known formulae have stronger hypotheses and, for the same α, they have m = 1/2 only. We also deduce a direct (error-free) generalization of Boas’ formula (Corollary 5). Furthermore, we give a modification of the main result for functions analytic in a domain and consider an extension to non-analytic functions as well. Finally, we illustrate the power of the method by examples.

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E-mail address: schmeisser@mi.uni-erlangen.de.
1. Introduction and discussion of some known methods

For $s \in \mathbb{N}$, we consider differentiation formulae of the form

$$f^{(s)}(x) = \sum_{n=1}^{N} A_n f(x_n) + R_{s,N}[f]$$

with nodes $x_1, \ldots, x_N$ and a remainder or error $R_{s,N}[f]$. When the number of nodes and their location is fixed, then the accuracy of such a formula is limited. On the other hand, if $N \geq s+1$ and the nodes are allowed to be arbitrarily close to $x$, then any desired accuracy is possible. However, if the nodes are all close to $x$, then the phenomenon of subtractive cancellation [19, pp. 502–504] can occur and will amplify possible errors due to computations with mantissas of finite length. The average distance of the nodes from $x$, denoted by

$$d^* := \frac{1}{N} \sum_{n=1}^{N} |x - x_n|,$$

may serve as an indicator for possible instabilities of this kind. When we compare certain classes of formulae, we will look at the values of $N$ and $d^*$ that are needed for obtaining a certain accuracy. It is desirable that $N$ is not too large and $d^*$ is not too small.

In many applications the location of the nodes is chosen relatively to $x$. Then it is enough to construct formulae for $x = 0$ and apply them to the function $f(\cdot + x)$. We will therefore restrict ourselves to $x = 0$ in this paper.

In order to put our results in perspective, we briefly discuss three of the most frequently used types of differentiation formulae.

1.1. Finite difference formulae

The simplest and most natural way of numerical differentiation is to approximate derivatives by divided differences. A systematic and more general approach of this kind consists in differentiating an interpolation polynomial. In view of Newton’s interpolation formula, the resulting approximation can be expressed in terms of divided differences.

In the simple case of $N$ equidistant nodes, the sequence of interpolation polynomials does, in general, not converge as $N \to \infty$; see [8, Chapter 4] or [20]. Therefore $N$ should be kept relatively small. This forces $d^*$ to be small which in turn will cause subtractive cancellations. In this dilemma only calculations in multiple precision can help to some extent.

Alternatively, one may care for optimally located nodes. The nodes

$$x_n := \cos \left( \frac{n \pi}{N} \right) \quad (n = 0, \ldots, N)$$

guarantee convergence for sufficiently smooth functions $f$ and, in addition, the corresponding number $d^*$ is bounded from below by a positive number for all $N \in \mathbb{N}$. For references, see [9,13,20,29] in the case of the first derivative and [14] for higher derivatives.

1.2. The method of contour integration

Let $f$ be analytic in a region that contains a disk of radius $r$ centered at the origin, and let $C$ be the positively oriented boundary of that disk. Then, by the generalized Cauchy
integral formula,

\[ f^{(s)}(0) = \frac{s!}{2\pi} \int_{C} \frac{f(z)}{z^{s+1}} \, dz = \frac{s!}{2\pi} \int_{0}^{2\pi} \frac{f(re^{it})}{(re^{it})^s} \, dt. \]

The integrand on the right-hand side is an infinitely differentiable periodic function. Therefore the trapezoidal rule is a best possible quadrature formula for approximating the integral. It coincides with the Euler–Maclaurin formula in this case. Thus we obtain

\[ f^{(s)}(0) = \frac{s!}{N} \sum_{n=1}^{N} \frac{f(re^{2\pi in/N})}{(re^{2\pi in/N})^s} + R_{s,N}[f]. \]

For estimates of \( R_{s,N}[f] \), see [12, 21, 22]. Here a favorable property is that always \( d^* = r \). For increasing the accuracy, \( N \) must be increased.

The hypothesis on \( f \) is much stronger than in the case of finite difference methods. In practice, this is not really a disadvantage since most of the functions occurring in applications are locally analytic. However, an extension of a real-valued function from an interval to a region in the complex plane can need a lot of efforts and may lead to complicated expressions. This is probably the main disadvantage of this type of formulae.

### 1.3. Sampling methods

Let us first introduce some terminology. A function \( f \) is an **entire function of exponential type** \( \sigma \), if \( f \) is analytic in the whole complex plane and satisfies the asymptotic growth condition

\[ \limsup_{r \to \infty} \frac{\log \max_{|z|=r} |f(z)|}{r} \leq \sigma. \]

The **Bernstein space** \( B^{p}_{\sigma} \) consists of all entire functions of exponential type \( \sigma \) whose restriction to \( \mathbb{R} \) belongs to \( L^{p}(\mathbb{R}) \) when \( p \in [1, \infty) \) and is bounded when \( p = \infty \); see [15, §6.1]. We have

\[ B^{1}_{\sigma} \subset B^{p}_{\sigma} \subset B^{r}_{\sigma} \subset B^{\infty}_{\sigma} \quad (1 \leq p \leq r \leq \infty). \]

An important member of \( B^{2}_{\sigma} \) is the sinc function defined by

\[ \text{sinc} z := \begin{cases} \sin \frac{\pi z}{\pi z} & \text{if } z \in \mathbb{C} \setminus \{0\}, \\ 1 & \text{if } z = 0. \end{cases} \]

The classical sampling theorem of Whittaker–Kotel’nikov–Shannon (see [23, p. 49]) says that for \( \sigma > 0 \) and \( h \in (0, \pi/\sigma) \), every \( f \in B^{2}_{\sigma} \) can be represented as

\[ f(z) = \sum_{n=-\infty}^{\infty} f(hn)\text{sinc}(h^{-1}z - n) \quad (z \in \mathbb{C}). \tag{2} \]

The series converges absolutely and uniformly on strips of finite width parallel to the real axis. It can be shown [6, §3.2] that differentiation inside the summation is admissible. Hence

\[ f^{(s)}(z) = \sum_{n=-\infty}^{\infty} f(hn) \frac{d^s}{dz^s} \left[ \text{sinc}(h^{-1}z - n) \right] \quad (z \in \mathbb{C}). \tag{3} \]
For numerical differentiation, this formula has two disadvantages:

(i) Unless \(|f|\) decays rapidly on the real line, the series in (3) converges slowly. Hence, when we construct a formula of the form (1) by truncating the series, we have to choose \(N\) very large.

(ii) The hypotheses on \(f\) are much stronger than in the aforementioned formulae. In practice, quite often functions will occur which do not belong to a Bernstein space.

However, both disadvantages can be considerably diminished by modifying (3) appropriately. If \(\varepsilon \in (0, \pi - h\sigma)\) and \(\Phi \in B^2_\varepsilon\) such that \(\Phi(0) = 1\), then

\[
f^{(s)}(z) = \sum_{n=-\infty}^{\infty} f(hn) \frac{d^s}{dz^s} \left[ \Phi(h^{-1}z - n) \text{sinc}(h^{-1}z - n) \right],
\]

(4)

see, e.g., [7,17,27]. By choosing a function \(\Phi\) whose modulus decays rapidly on \(\mathbb{R}\), the convergence of the series in (4) can be much accelerated. It was shown in [10] that for \(x > 1\) there exists a function \(\Phi\) of the desired form such that

\[
\Phi(x) = O\left( \exp\left( - \frac{|x|}{(\log |x|)^2} \right) \right) \quad (x \to \pm \infty).
\]

This is nearly the best one can have. For a function in \(B^2_\varepsilon\) a decay like \(O(e^{-x|x|})\) with a positive \(x\) is not possible. Therefore, Qian [24] left the Bernstein spaces and considered a scaled form of the Gaussian function \(e^{-x^2/2}\) as a multiplier \(\Phi(x)\). Then (4) is no longer true; it only holds with an error term. Fortunately, this additional error can be kept so small that the truncated series in (4) with \(2N + 1\) terms approximates \(f^{(s)}\) with a total error which is for \(h \in (0, \pi/\sigma)\) and \(\varepsilon := (\pi - h\sigma)/2\) bounded by

\[
M_s e^{-\varepsilon N} \frac{e^{-2N}}{N^{1/2}}.
\]

(5)

The number \(M_s\) depends on \(f, h, s\) but not on \(N\). Moreover,

\[
d^* = h \frac{N(N + 1)}{2N + 1}.
\]

Since \(h\) can be fixed while \(N\) is increased for increasing the accuracy, there is no danger of instability. Also note that, other than in the method of contour integration, we do not need the analytic extension of \(f\) into the complex plane in computations.

The bound (5) for the error of an approximation of \(f^{(s)}\) by \(2N + 1\) successive values \(f(nh)\) and with \(\varepsilon\) as before can also be extracted from papers by Qian–Creamer [25] and Qian–Ogawa [26] in which variants of (2) were the starting point.

The formulae (3), (4) and modifications have also been used for approximating the derivatives of functions that do not belong to a Bernstein space. Stenger [31, §3.5, §4.4] has results for functions analytic in a strip or, more generally, in a simply connected region. Butzer and Stens [7] and Butzer et al. [6, Section 4.4] have results for functions defined on \(\mathbb{R}\) but not necessarily analytic. Bulychev and Burlaj [5] considered functions given on an interval of finite length, extended them to \(\mathbb{R}\) by a regularizing procedure and applied (3).
In the next section, we consider an interpolation formula of R.P. Boas for the first derivative of a function \( f \in B_\alpha^\infty \); see Theorem A and note that equivalently, 

\[
\frac{h}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{(2n-1)^2} \left[ f(h(2n-1)) - f(-h(2n-1)) \right].
\] (6)

This formula may be classified as a sampling method since it can be deduced from (2) although it has some advantages over (3) for \( s = 1 \). We will improve (6) in two ways, by incorporating a Gaussian multiplier and by extending it to higher derivatives. The resulting differentiation formula for the derivative of order \( s \) has \( N' \) nodes and works for all entire functions of exponential type, including those that grow exponentially on the real line. It has an error bound 

\[
M_s \frac{e^{-2N}}{N^m},
\]

where \( \alpha > 0 \) and \( m = 3/2 \), \( N' = 2N \) for odd \( s \) while \( m = 5/2 \), \( N' = 2N + 1 \) for even \( s \). Again, the number \( M_s \) depends on \( f, h \) and \( s \) but not on \( N \). Furthermore, for functions in \( B_\alpha^\infty \) the number \( \alpha \) is the same as in (5) when the nodes are spaced in the same way.

For \( s = 1 \) and 2, these formulae take the form

\[
f'(0) = \frac{2}{\pi h} \sum_{n=1}^{N} \frac{(-1)^{n+1}}{(2n-1)^2} e^{-\omega(2n-1)^2} \left[ f(h(2n-1)) - f(-h(2n-1)) \right]
\]

\[
+ \frac{1}{h} R_{1,N}[f],
\] (7)

\[
f''(0) = \frac{4}{\pi h^2} \sum_{n=1}^{N} \frac{(-1)^{n+1}}{(2n-1)^3} e^{-\omega(2n-1)^2} \left[ f(h(2n-1)) - 2f(0) + f(-h(2n-1)) \right]
\]

\[
+ \frac{2}{h^2} R_{2,N}[f].
\] (8)

The value of \( \omega \) is specified in Lemma 1. Furthermore, representations and estimates for \( R_{s,N}[f] \) are given in Theorem 2. It is remarkable that in all formulae for a derivative of odd order \( s \), the dependence on \( f \), as shown by the term in square brackets, and the Gaussian multiplier are the same as in (7). The other factors constitute an expression \( A_{s,N}[f] \), say, that depends on \( s \) and decays like \( (2n-1)^{-2} \) with increasing \( |n| \). Analogously, all the formulae for a derivative of even order have the same structure as (8) with the corresponding \( A_{s,N}[f] \) decaying like \( (2n-1)^{-3} \).

In Section 3, we modify our differentiation formula for functions analytic in a domain. In Section 4, we study a modification for a class of functions which are not necessarily analytic. Finally, in Section 5, we illustrate the results by numerical examples.

2. Boas type formulae for entire functions of exponential type

The result of Boas [2, formula (6)] that inspired the approach to numerical differentiation considered in the present paper may be stated as follows.

**Theorem A.** Let \( f \in B_\alpha^\infty \), where \( \sigma > 0 \). Then, for \( 0 < h \leq \frac{\pi}{2\sigma} \), we have

\[
hf'(0) = \frac{2}{\pi} \sum_{n=-\infty}^{\infty} \frac{(-1)^{n+1}}{(2n-1)^2} f(h(2n-1)).
\] (9)
Boas proved (9) by representing \( f' \) by a Stieltjes integral and expanding the kernel of this integral in a Fourier series. Browder [4] gave a proof by contour integration. Besides, (9) can be deduced from the classical sampling theorem [16, pp. 337–338]. Clearly, (9) applies to trigonometric polynomials. In this case, the series on the right-hand side can be reduced to a finite sum, which yields an interpolation formula discovered earlier by Riesz [28]. For this reason, (9) has also been called the generalized Riesz interpolation formula.

For deducing the announced improvement of Theorem A, we will proceed in two steps, using the partial result of the first step as a lemma.

As usual, we denote by \( \lfloor x \rfloor \), where \( x \in \mathbb{R} \), the largest integer not exceeding \( x \). Furthermore, we introduce

\[
\begin{align*}
  c_j(\omega) &:= \sum_{v=0}^{j} \frac{(-\omega)^v}{v!} \left( \frac{\pi}{2} \right)^{2j-2v} \frac{|E_{2j-2v}|}{(2j-2v)!} \quad (j \in \mathbb{N}_0), \\
\end{align*}
\]

where \( E_{2j-2v} \) are the Euler numbers; see [1, Chapter 23] or [11, §9.63].

**Lemma 1.** Let \( f \) be an entire function such that

\[
|f(x + iy)| \leq \phi(|x|)e^{\sigma|y|} \quad (x, y \in \mathbb{R}),
\]

where \( \phi \) is a non-decreasing, non-negative function on \([0, \infty)\) and \( \sigma > 0 \). Then, for \( h \in (0, \pi/(2\sigma)) \), \( \alpha := \pi/2 - \sigma, N \in \mathbb{N} \), and \( \omega := \alpha/(4N) \), we have

\[
\begin{align*}
  \sum_{j=0}^{[s/2]} c_j(\omega) h^{s-2j} f^{(s-2j)}(0) & = \frac{2}{\pi} \sum_{n=-N+1}^{N} \frac{(-1)^n+1}{(2n-1)(2n+1)^{1/2}} e^{-\omega(2n-1)^2} f(h(2n - 1)) + r_{s,N}[f] \\
\end{align*}
\]

with a remainder satisfying

\[
|r_{s,N}[f]| \leq \frac{e^{-2N} \phi(2hN)}{\sqrt{2\pi} 2^{s-1} N^{s+1/2}} \beta_N,
\]

where

\[
\beta_N := \min \left\{ 2.14, \frac{1}{1 - e^{-2\pi N}} + \frac{2}{\sqrt{2\pi N}} \right\} = 1 + O \left( N^{-1/2} \right) \quad (N \to \infty).
\]

**Proof.** We may assume that \( \sigma < \pi/2 \) and \( h = 1 \) since the more general result can be deduced from that special case by considering the function \( z \mapsto f(hz) \).

Let us introduce

\[
\begin{align*}
  K_s(z) &:= \frac{e^{-\omega z^2} f(z)}{z^{s+1} \cos(\pi z/2)}. \\
\end{align*}
\]

This is a meromorphic function with simple poles at \( z = 2n - 1 \) for \( n \in \mathbb{Z} \) and a pole of multiplicity at most \( s + 1 \) at the origin. For the residues at the simple poles, we readily find that

\[
\text{res} \left( K_s; 2n - 1 \right) = \frac{2}{\pi} \cdot \frac{(-1)^n}{(2n - 1)^{s+1}} e^{-\omega(2n-1)^2} f(2n - 1).
\]
For the residue at the origin, a standard formula yields that
\[
\text{res } (K_s; 0) = \frac{1}{s!} \left[ \frac{d^s}{dz^s} \frac{e^{-\omega z^2}}{\cos(\pi z/2)} f(z) \right]_{z=0}.
\]
Introducing the auxiliary function
\[
g(z) := \frac{e^{-\omega z^2}}{\cos(\pi z/2)}
\]
and noting that \(g\) is an even function, we find by Leibniz’ rule
\[
\text{res } (K_s; 0) = \sum_{j=0}^{[s/2]} g^{(2j)}(0) \cdot \frac{f^{(s-2j)}(0)}{(2j)! (s-2j)!}.
\]
(15)
Again, Leibniz’ rule can be employed for calculating the derivatives of \(g\) from those of \(e^{-\omega z^2}\) and \(1/\cos(\pi z/2)\). The latter are both even functions, and so we need their derivatives of even order only.
It follows from standard properties of the Hermite polynomials \(H_n\), see, e.g., [1, Chapter 22] or [11, §8.95], that
\[
\frac{d^{2\nu}}{dz^{2\nu}} e^{-\omega z^2} = \omega^\nu H_{2\nu}(\omega^{1/2} z) e^{-\omega z^2},
\]
which gives
\[
\left[ \frac{d^{2\nu}}{dz^{2\nu}} e^{-\omega z^2} \right]_{z=0} = \omega^\nu H_{2\nu}(0) = (-\omega)^\nu \frac{(2\nu)!}{\nu!}.
\]
(16)
Next, using the expansion [11, formula 1.4119]
\[
\frac{1}{\cos z} = \sum_{k=0}^\infty \frac{|E_{2k}|}{(2k)!} z^{2k},
\]
we see that
\[
\left[ \frac{d^{2j-2\nu}}{dz^{2j-2\nu}} \frac{1}{\cos(\pi z/2)} \right]_{z=0} = \left( \frac{\pi}{2} \right)^{2j-2\nu} |E_{2j-2\nu}|.
\]
(17)
The formulae (16) and (17) allow us to conclude that
\[
g^{(2j)}(0) \cdot \frac{f^{(s-2j)}(0)}{(2j)!} = \sum_{\nu=0}^{j} \frac{(-\omega)^\nu}{\nu!} \left( \frac{\pi}{2} \right)^{2j-2\nu} |E_{2j-2\nu}|.
\]
Combined with (15), we obtain
\[
\text{res } (K_s; 0) = \sum_{j=0}^{[s/2]} c_j(\omega) \frac{f^{(s-2j)}(0)}{(s-2j)!}
\]
with \(c_j(\omega)\) defined by (10).
Now let $\mathcal{R}$ be the positively oriented rectangle with vertices at $\pm 2N \pm i2N$. Then the residue theorem for the function $K_s$ shows that (12) holds for $h = 1$ with

$$ r_{s,N}[f] = \frac{1}{2\pi i} \int_{\mathcal{R}} K_s(z) \, dz. \quad (18) $$

It remains to estimate the right-hand side.

Denote by $I_{\text{hor}}^\pm$ the contributions to the right-hand side of (18) coming from the two horizontal parts of $\mathcal{R}$, where $+$ and $-$ refer to the upper and lower line segment, respectively. Similarly, denote by $I_{\text{vert}}^\pm$ the contributions coming from the two vertical parts of $\mathcal{R}$, where $+$ and $-$ refer to the right and left line segment, respectively. Then

$$ r_{s,N}[f] = I_{\text{hor}}^- + I_{\text{hor}}^+ + I_{\text{vert}}^+ + I_{\text{vert}}^-, \quad (19) $$

where

$$ I_{\text{hor}}^\pm = \frac{\pm 1}{2\pi i} \int_{-2N}^{2N} \frac{e^{-\omega(t \pm i2N)^2} f(t \pm i2N)}{(t \pm i2N)^{s+1} \cos(\pi(t \pm i2N)/2)} \, dt $$

and

$$ I_{\text{vert}}^\pm = \frac{\pm 1}{2\pi} \int_{-2N}^{2N} \frac{e^{-\omega(\pm 2N + it)^2} f(\pm 2N + it)}{(\pm 2N + it)^{s+1} \cos(\pi(\pm 2N + it)/2)} \, dt. $$

In order to estimate these integrals, we use the following inequalities holding for $x, y \in \mathbb{R}$ and $t \in [-2N, 2N]$

$$ |e^{-(x+iy)^2}| \leq e^{-x^2} e^{y^2}, \quad (20) $$

$$ |\cos(\pi(t \pm i2N)/2)| \geq \sinh(\pi N) = \frac{e^\pi N}{2} \left( 1 - e^{-2\pi N} \right), \quad (21) $$

$$ |\cos(\pi(\pm 2N + it)/2)| = \cosh(\pi t/2) \geq \frac{e^{\pi |t|/2}}{2}, \quad (22) $$

$$ |t \pm i2N|^{s+1} \geq (2N)^{s+1}, \quad |\pm 2N + it|^{s+1} \geq (2N)^{s+1}, \quad (23) $$

and

$$ |f(t \pm i2N)| \leq \phi(2N) e^{2\sigma N}, \quad |f(\pm 2N + it)| \leq \phi(2N) e^{\sigma |t|}. \quad (24) $$

With these relations, we find that

$$ |I_{\text{hor}}^\pm| \leq \frac{e^{-(\pi-2\sigma)N+4\sigma N^2}}{\pi(1 - e^{-2\pi N}) \cdot (2N)^{s+1}} \int_{-2N}^{2N} e^{-\omega t^2} \, dt $$

$$ \leq \frac{e^{-\sigma N} \phi(2N)}{\pi(1 - e^{-2\pi N}) \cdot (2N)^{s+1}} \int_{-\infty}^{\infty} e^{-\omega t^2} \, dt $$

$$ = \frac{e^{-\sigma N} \phi(2N)}{\sqrt{2\pi} 2^s N^{s+1/2} \cdot 1 - e^{-2\pi N}}. \quad (25) $$
For the contributions coming from the vertical parts of $\mathcal{R}$, we obtain

$$|I_{\text{vert}}^\pm| \leq e^{-\frac{4\sigma N^2}{\pi (2N)^{s+1}}} \int_{-2N}^{2N} e^{-\frac{1}{4}(\pi^2/2-\sigma)|t|+\omega t^2} \, dt = e^{-\frac{2N}{\pi 2^s N^{s+1}}} \int_{-2N}^{2N} e^{-\omega t^2} \, dt.$$  

It is easily seen that

$$\int_{2N}^{-2N} e^{-\omega t^2} \, dt \leq \int_{0}^{2N} e^{-t^2/2} \, dt < \frac{2}{\sqrt{\pi}}. \tag{26}$$

Clearly, the integral on the left-hand side is also bounded by $2N$. Thus, taking the geometric mean of these two bounds, we have

$$\int_{2N}^{-2N} e^{-\omega t^2} \, dt \leq 2 \sqrt{\frac{N}{\pi}}. \tag{27}$$

Hence, using (26) and (27) alternatively, we obtain

$$|I_{\text{vert}}^\pm| \leq e^{-\frac{2N}{\pi \sqrt{2^s-1} N^{s+1}}} \text{ and } |I_{\text{vert}}^\pm| \leq \frac{e^{-\frac{2N}{\pi \sqrt{2^s-1} N^{s+1}}}}{\sqrt{\pi}}. \tag{28}$$

Combining (19), (25), and (28), we find that (13) holds with

$$\beta_N \leq \frac{1}{1-e^{-2\pi N}} + \frac{2}{\sqrt{\pi} \sqrt{2^s-1} N} \text{ and } \beta_N \leq \frac{1}{1-e^{-2\pi}} + \frac{2}{\sqrt{\pi}} < 2.14.$$ 

Now the proof is easily completed. \( \square \)

Lemma 1 provides a differentiation formula of the desired form for $s = 1$ and 2 only. For larger $s$, further derivatives of lower order appear on the left-hand side of (12). However, we can eliminate these additional derivatives by using (12) recursively.

For this aim, let us first introduce some notation. Employing the numbers (10), we define

$$a_0(\omega) := 1, \quad a_j(\omega) := -\sum_{\ell=1}^{j} c_\ell(\omega) a_{j-\ell}(\omega) \quad (j \in \mathbb{N}). \tag{29}$$

An explicit form of these quantities is

$$a_j = (-1)^j \det \begin{pmatrix} c_1 & 1 \\ c_2 & c_1 & 1 \\ \vdots & \vdots & \vdots & \ddots \\ c_{j-1} & c_{j-2} & c_{j-3} & \cdots & 1 \\ c_j & c_{j-1} & c_{j-2} & \cdots & c_1 \end{pmatrix} \quad (j \in \mathbb{N}),$$

where we have suppressed the argument $\omega$ on both sides. Next we introduce the polynomials

$$P_s(\omega; z) := \sum_{j=1}^{s} a_{s-j}(\omega) z^j \quad (s \in \mathbb{N}). \tag{30}$$

Finally, we define

$$\delta_n f_h := f(h(2n-1)) - f(-h(2n-1)), \quad \delta_n^2 f_h := f(h(2n-1)) - 2f(0) + f(-h(2n-1)). \tag{31}$$
**Theorem 2.** Let \( s \in \mathbb{N} \). Under the hypotheses of Lemma 1 and in the previous notation, there exists a sequence \((\gamma_j)_{j \in \mathbb{N}}\) of absolute constants such that the following holds:

(i) For derivatives of odd order, we have

\[
\frac{h^{2s-1} f^{(2s-1)}(0)}{(2s-1)!} = \frac{2}{\pi} \sum_{n=1}^{N} (-1)^{n+1} P_s \left( \omega; (2n-1)^{-2} \right) e^{-\omega(2n-1)^2} \delta_n f_h + R_{2s-1,N}[f],
\]

where

\[
R_{2s-1,N}[f] = \sum_{j=1}^{s} a_{s-j}(\omega) r_{2j-1,N}[f]
\]

and

\[
\left| R_{2s-1,N}[f] \right| \leq \gamma_{2s-1} \cdot \frac{e^{-2N} \phi(2hN)}{\sqrt{\pi N}}. \tag{32}
\]

(ii) For derivatives of even order, we have

\[
\frac{h^{2s} f^{(2s)}(0)}{(2s)!} = \frac{2}{\pi} \sum_{n=1}^{N} (-1)^{n+1} P_s \left( \omega; (2n-1)^{-2} \right) \frac{e^{-\omega(2n-1)^2}}{2n-1} \delta_n^2 f_h + R_{2s,N}[f],
\]

where

\[
R_{2s,N}[f] = \sum_{j=1}^{s} a_{s-j}(\omega) r_{2j,N}[f - f(0)]
\]

and

\[
\left| R_{2s,N}[f] \right| \leq \gamma_{2s} \cdot \frac{e^{-2N} \phi(2hN)}{\sqrt{\pi N}}. \tag{33}
\]

**Proof.** We shall proceed by induction on \( s \). Let us first turn to statement (i).

For \( s = 1 \), the conclusion follows from (12) and (13). Now assume that statement (i) holds for derivatives of order 1, 3, \ldots, 2s − 1. For \( s \) replaced by \( 2s + 1 \), we may rewrite (12) as

\[
\frac{h^{2s+1} f^{(2s+1)}(0)}{(2s+1)!} = - \sum_{j=1}^{s} c_j(\omega) \frac{h^{2s+1-2j} f^{(2s+1-2j)}(0)}{(2s + 1 - 2j)!} + \frac{2}{\pi} \sum_{n=1}^{N} \frac{(-1)^{n+1}}{(2n-1)^{2s+2}} e^{-\omega(2n-1)^2} \delta_n^2 f_h + R_{2s+1,N}[f]. \tag{34}
\]

By the induction hypothesis

\[
\frac{h^{2s+1-2j} f^{(2s+1-2j)}(0)}{(2s + 1 - 2j)!} = \frac{2}{\pi} \sum_{n=1}^{N} (-1)^{n+1} P_{s-j+1} \left( \omega; (2n-1)^{-2} \right) e^{-\omega(2n-1)^2} \delta_n f_h + R_{2s+1-2j,N}[f] \quad (j = 1, \ldots, s).
\]

Substituting this in (34), we find that the desired formula for \( f^{(2s+1)}(0) \) holds provided that

\[
P_{s+1}(\omega; z) = z^{s+1} - \sum_{j=1}^{s} c_j(\omega) P_{s+1-j}(\omega; z)
\]
and

\[ R_{2s+1,N}[f] = r_{2s+1,N}[f] - \sum_{j=1}^{s} c_j(\omega) R_{2s+1-2j,N}[f]. \]

These equations are indeed satisfied as a consequence of (29), (30), and the induction hypothesis applied to \( R_{2s+1-2j,N}[f] \).

It remains to prove (33). First we note that \(|\omega| \leq \pi/8\). Hence (10) shows that each \(|c_j(\omega)|\) is bounded by an absolute constant and, as a consequence of (29), each \(|a_j(\omega)|\) is also bounded by an absolute constant. Furthermore, each \(|r_{2j-1,N}[f]|\) can be estimated according to (13) with \( \beta_N \) replaced by 2.14. With these indications, it is readily seen that (33) follows from (32). This completes the proof of statement (i).

We now turn to statement (ii). For \( s \) replaced by 2\( s \) and \( f \) replaced by \( f - f(0) \), formula (12) may be rewritten as

\[
\frac{h^{2s} f^{(2s)}(0)}{(2s)!} = -\sum_{j=1}^{s-1} c_j(\omega) \frac{h^{2s-2j} f^{(2s-2j)}(0)}{(2s - 2j)!} + \frac{2}{\pi} \sum_{n=1}^{N} \frac{(-1)^{n+1}}{(2n - 1)^{2s+1}} e^{-\omega(2n-1)^2/\beta_n^2} \phi_n^2 + r_{2s,N}[f - f(0)].
\]

It should also be noted that the right-hand side of (13) with \( s \) replaced by 2\( s \) and then multiplied by 2 is certainly a bound for \(|r_{2s,N}[f - f(0)]|\). With these modifications of the conclusions of Lemma 1, the proof of statement (ii) becomes analogous to that of statement (i). It does not seem necessary to present details.

Apart from the higher accuracy and the weaker assumptions on \( f \), another advantage of the formulae of Theorem 2 as compared to those in [24] or [25] is that they can be easily established in explicit form. Only the polynomials \( P_s(\omega; z) \) have to be calculated, which is not difficult. For example, for the formula for the fourth derivative, we only need \( P_2(\omega; z) \), which is easily seen to be

\[
z^2 - \left( \frac{\pi^2}{8} - \omega \right) z.
\]

On the other hand, the calculation of the corresponding formula in [24] is already a very laborious task.

It may be surprising that in Theorem 2 we did not require that \( f \) is of exponential type; in particular, we did not impose any restrictions on the growth of \( \phi \) which is a majorant for \( f \) on \( \mathbb{R} \). However, if \( f \) is not of exponential type, then the error bounds of Theorem 2 may not approach zero as \( N \to \infty \).

Every entire function \( f \) of exponential type can be estimated as

\[
|f(x + iy)| \leq M e^{K|x|+\sigma|y|} \quad (x, y \in \mathbb{R})
\]

with non-negative numbers \( M, K, \) and \( \sigma \). Conversely, every entire function \( f \) that satisfies (35) is of exponential type \( (K^2 + \sigma^2)^{1/2} \).

For \( c > 0 \), we shall say that an error bound converges to zero \emph{exponentially of order} \( c \) as \( N \to \infty \) if it converges at least as fast as \( M e^{-cN} \) for some non-negative \( M \). In the following
Corollary, it is remarkable that the error bounds converge exponentially for any entire function of exponential type, including those that grow exponentially along the real line, provided that we restrict \( h \) appropriately.

**Corollary 3.** Let \( f \) be an entire function satisfying (35) with non-negative numbers \( M, \kappa, \) and \( \sigma \). Then the conclusions of Theorem 2 hold with \( \phi(x) := Me^{kx} \). For \( h \in (0, \pi/(2\sigma + 4\kappa)) \), we have exponential convergence of order \( x - 2h\kappa \).

While exponential growth of \( f \) along the real line, as it may occur if (35) holds with a positive \( \kappa \), reduces the order of exponential convergence from \( x \) to \( x - 2h\kappa \), polynomial growth on \( \mathbb{R} \) does not reduce the order.

**Corollary 4.** Let \( f \) be an entire function of exponential type \( \sigma \) such that
\[
|f(x)| \leq M \left( 1 + x^2 \right)^{k/2} (x \in \mathbb{R}),
\]
where \( M \geq 0 \) and \( k \in \mathbb{N}_0 \). Then the conclusions of Theorem 2 hold with \( \phi(x) = 2^{k/2}M(x + 1)^k \).

**Proof.** We proceed as in the proof of [30, Corollary 2.3]. The function \( g \), defined by
\[
g(z) := \frac{f(z)}{(z + i)^k},
\]
is analytic and of exponential type \( \sigma \) in the closed upper half-plane. Moreover, \( |g(x)| \leq M \) for \( x \in \mathbb{R} \). Hence, by [3, Theorem 6.2.4], we have
\[
|g(x + iy)| \leq Me^{\sigma y} \quad (x, y \in \mathbb{R}, \ y \geq 0),
\]
and so
\[
|f(x + iy)| \leq M \left( x^2 + (|y| + 1)^2 \right)^{k/2} e^{\sigma|y|} \tag{38}
\]
for \( x \in \mathbb{R} \) and \( y \geq 0 \). An analogous consideration for the lower half-plane with \( i \) replaced by \(-i\) in (37) shows that (38) holds for all \( x, y \in \mathbb{R} \). Now, in the proof of Lemma 1, we needed \( f(x + iy) \) for \( |x| \leq 2N \) and \( |y| \leq 2N \) only; see (24). Under these restrictions, (38) gives
\[
|f(x + iy)| \leq M \left( (2N)^2 + (2N + 1)^2 \right)^{k/2} e^{\sigma|y|} < 2^{k/2}M(2N + 1)^k e^{\sigma|y|},
\]
which shows that the crucial estimates (24) hold for \( \phi(x) := 2^{k/2}M(x + 1)^k \) though (11) may not be true for this \( \phi \). It is also easily checked that \( \phi(h \cdot) \) will yield the corresponding estimates (24) for \( f(h \cdot) \). \( \square \)

Note that for functions \( f \in B^\infty_\sigma \), Corollary 4 applies with \( k = 0 \) and \( M := \|f\|_\infty \) being the supremum norm on \( \mathbb{R} \).

For theoretical and esthetical reasons, it may be interesting to have a direct generalization of the formula (9) without a remainder and with a series instead of a sum. Such a result is obtained by letting \( N \to \infty \).
Corollary 5. Let $f \in B_{\sigma}^\infty$, where $\sigma > 0$, and define

$$P_s^*(z) := \sum_{j=1}^s \frac{(-1)^{s-j}}{(2s - 2j)!} \left( \frac{\pi}{2} \right)^{2s-2j} z^j \quad (s \in \mathbb{N}).$$

Then, for $s \in \mathbb{N}$ and $0 < h \leq \pi/(2\sigma)$, we have

$$h^{2s-1} f^{(2s-1)}(0) \over (2s-1)! = \frac{2}{\pi} \sum_{n=-\infty}^{\infty} (-1)^{n+1} P_s^* \left( (2n - 1)^{-2} \right) f(h(2n - 1))$$  \hspace{1cm} (39)

and

$$h^{2s} f^{(2s)}(0) \over (2s)! = \frac{(-1)^s}{(2s)!} \left( \frac{\pi}{2} \right)^{2s} f(0) + \frac{2}{\pi} \sum_{n=-\infty}^{\infty} (-1)^{n+1} \frac{P_s^* \left( (2n - 1)^{-2} \right)}{2n - 1} f(h(2n - 1)).$$  \hspace{1cm} (40)

Proof. We only indicate a proof without working out all details. First suppose that $0 < h < \pi/(2\sigma)$. Then we conclude from Theorem 2 by letting $N \to \infty$ that

$$h^{2s-1} f^{(2s-1)}(0) \over (2s-1)! = \frac{2}{\pi} \sum_{n=-\infty}^{\infty} (-1)^{n+1} P_s \left( (2n - 1)^{-2} \right) \delta_n f_h$$  \hspace{1cm} (41)

and

$$h^{2s} f^{(2s)}(0) \over (2s)! = \frac{2}{\pi} \sum_{n=-\infty}^{\infty} (-1)^{n+1} \frac{P_s \left( (2n - 1)^{-2} \right)}{2n - 1} \delta_n^2 f_h.$$  \hspace{1cm} (42)

The uniform convergence of the series on the right-hand side allows us to extend these formulae to $h = \pi/(2\sigma)$.

Next we mention that

$$a_j(0) = \frac{(-1)^j}{(2j)!} \left( \frac{\pi}{2} \right)^{2j} \quad (j \in \mathbb{N}_0)$$

as can be proved with the help of the recurrence formula (29) and properties of the Euler numbers $[11, \$9.63, 9.65]$. Hence $P_s(0; z) \equiv P_s^*(z)$ for $s \in \mathbb{N}$. Now (39) is easily obtained by splitting the finite difference $\delta_n f_h$ in (41).

In order to prove (40), we have to split the second difference $\delta_n^2 f_h$ in (42). For this, it is enough to observe that the coefficient of $f(0)$, appearing as

$$-\frac{4}{\pi} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{P_s \left( (2n - 1)^{-2} \right)}{2n - 1},$$

can be calculated in closed form by setting $h = 1$ and applying (42) to $f(z) = \cos(\pi z/2)$. □
3. A modification for functions analytic in a domain

In the proof of Lemma 1, we needed the restriction of $f$ to a square only. This allows us to modify the formulae of Theorem 2 so that they apply to functions analytic in a square. However, while in Theorem 2 the numbers $h$ and $N$ can be chosen independently, they have now to be correlated. This is unavoidable since if the number of nodes increases and their location is restricted to a square, they must necessarily become denser.

For $d > 0$, we now introduce $Q_d := \{z \in \mathbb{C} : |\Re z| \leq d, |\Im z| \leq d\}$.

**Theorem 6.** Let $f$ be analytic in $Q_d$, and let $|f|$ be bounded by $M$. Then, in the notation of Theorem 2, the following statements hold for $s, N \in \mathbb{N}, h := d/(2N), \omega := \pi/(8N)$:

(i) For derivatives of odd order, we have

$$
\frac{h^{2s-1} f^{(2s-1)}(0)}{(2s-1)!} = \frac{2}{\pi} \sum_{n=1}^{N} (-1)^{n+1} P_s(\omega; (2n-1)^{-2}) e^{-\omega(2n-1)^2} \delta_n f_h + R_{2s-1,N}[f],
$$

where

$$
R_{2s-1,N}[f] = \sum_{j=1}^{s} a_{s-j}(\omega) \rho_{2j-1,N}
$$

with

$$
|\rho_{2s-1,N}| \leq \frac{8M}{\pi} \cdot \frac{e^{-\pi N/2}}{(2N)^{2j-1/2}}
$$

and

$$
R_{2s-1,N}[f] = O\left(\frac{e^{-\pi N/2}}{N^{3/2}}\right) \quad (N \to \infty).
$$

(ii) For derivatives of even order, we have

$$
\frac{h^{2s} f^{(2s)}(0)}{(2s)!} = \frac{2}{\pi} \sum_{n=1}^{N} (-1)^{n+1} P_s(\omega; (2n-1)^{-2}) e^{-\omega(2n-1)^2} \frac{\delta_n^2 f_h}{2n-1} + R_{2s,N}[f],
$$

where

$$
R_{2s,N}[f] = \sum_{j=1}^{s} a_{s-j}(\omega) \rho_{2j,N}
$$

with

$$
|\rho_{2j,N}| \leq \frac{16M}{\pi} \cdot \frac{e^{-\pi N/2}}{(2N)^{2j+1/2}}
$$

and

$$
R_{2s,N}[f] = O\left(\frac{e^{-\pi N/2}}{N^{5/2}}\right) \quad (N \to \infty).
$$
Proof. Let \( N \in \mathbb{N} \) be arbitrary but fixed for the moment. Then, apart from the asymptotic formulae, it suffices to prove the statements for \( Q_{2N} \) since they will follow for arbitrary \( Q_d \) by considering the function \( z \mapsto f(zd/(2N)) \).

Obviously, for \( Q_{2N} \), the proof of Lemma 1 applies with \( \phi(x) \equiv M, \sigma = 0, \alpha = \pi/2 \), and \( \omega = \pi/(8N) \). It yields that the conclusions of Lemma 1 hold for \( h = 1 \) with

\[
|r_{s,N}[f]| \leq \frac{4Me^{-\pi N/2}}{(2N)^{1/2} \beta_N}.
\]

Since \( \alpha = \pi/2 \), it is seen that the minimum defining \( \beta_N \) is strictly less than 2. We may therefore replace \( \beta_N \) by 2 in (43).

Writing \( \rho_{2j-1,N} \) for \( r_{2j-1,N}[f] \) and \( \rho_{2j,N} \) for \( r_{2j,N}[f - f(0)] \), we obtain the differentiation formulae and the representations of their remainders exactly in the same way as in the proof of Theorem 2.

After having transformed these results from \( Q_{2N} \) to \( Q_d \), we need not keep \( N \) fixed any more. Now the asymptotic formulae for the remainders are easily deduced. \( \square \)

Remark 7. The formulae of Theorem 6 can be transformed to more general domains. Let \( f \) be analytic in a domain \( \mathcal{G} \) that contains the origin. Let \( \psi \) be a conformal mapping which maps \( Q_d \) onto a subset of \( \mathcal{G} \) such that \( \psi(0) = 0 \). If \( |f| \) is bounded on \( \psi(Q_d) \), then we can apply Theorem 6 to \( g := f \circ \psi \). The derivative of order \( s \) of \( g \) at 0 is a linear combination of \( f'(0), f''(0), \ldots, f^{(s)}(0) \). In order to obtain an explicit formula for \( f^{(s)}(0) \), we can eliminate the derivatives of lower order by proceeding as in the proof of Theorem 2. An example is presented in Section 5; see Example 14.

4. A modification extending to non-analytic functions

The differentiation formulae of Theorem 2 involve \( \sigma, h, \) and \( N \). While in the last section we correlated \( h \) and \( N \) by setting \( h := d/(2N) \), we now correlate \( \sigma \) and \( h \) by setting \( h := \pi/(4\sigma) \) which implies \( \omega = \pi/(16N) \). The resulting functional for approximating the derivative of order \( s \) at 0 shall be denoted by \( D_{h,N}^{[2s]} \), that is,

\[
D_{h,N}^{[2s]}[f] := \frac{2(2s)!}{\pi h^{2s}} \sum_{n=1}^{N} (-1)^{n+1} P_s \left( \omega; (2n - 1)^{-2} \right) e^{-\omega(2n-1)^2} \delta_n f_h,
\]

\[
D_{h,N}^{[2s+1]}[f] := \frac{2(2s+1)!}{\pi h^{2s+1}} \sum_{n=1}^{N} (-1)^n P_{s+1} \left( \omega; (2n - 1)^{-2} \right) e^{-\omega(2n-1)^2} \delta_n^2 f_h.
\]

We want to apply these functionals to functions \( f \) that are not necessarily analytic. More precisely, we consider a class of functions that was used by Butzer and Stens in [7]. For this, we recall the following notation.

Let \( C_B(\mathbb{R}) \) be the class of all functions \( f : \mathbb{R} \to \mathbb{C} \) that are uniformly continuous and bounded on \( \mathbb{R} \). For \( f \in C_B(\mathbb{R}) \) and \( \delta > 0 \), define

\[
\omega_2(f; \delta) := \sup_{|h| \leq \delta} \|f(\cdot + h) - 2f(\cdot) + f(\cdot - h)\|_\infty.
\]

Finally, for \( \kappa > 0 \), we introduce the Lipschitz class

\[
\text{Lip}_2(\kappa) := \{ f \in C_B(\mathbb{R}) : \omega_2(f; \delta) = O(\delta^\kappa) \text{ as } \delta \to 0_+ \}.
\]
Theorem 8. For \( m \in \mathbb{N} \) and \( \kappa \in [0, 1] \), let \( f \in C_B(\mathbb{R}) \) be \( m \) times differentiable such that \( f^{(m)} \in \text{Lip}_2(\kappa) \). Then, for \( s \in \mathbb{N} \), \( s \leq m \),

\[
N := \max \left\{ 1, \left\lfloor -\frac{4}{\pi} (m + \kappa) \log h \right\rfloor \right\}
\]

and \( \omega = \pi/(16N) \), we have

\[
\left| f^{(s)}(0) - D^{[s]}_{h,N}[f] \right| = O \left( h^{m+\kappa-s} \right) \quad (h \to 0_+).
\]

Proof. We adopt ideas from a paper of Butzer and Stens [7, Section 3]. For \( \sigma > 0 \), we associate with \( f \) a function \( F_\sigma \in B^\infty_\sigma \) which is the best approximation to \( f \) with respect to the norm \( \| \cdot \|_\infty \). Then

\[
\left| f^{(s)}(0) - D^{[s]}_{h,N}[\sigma f] \right| \leq \left| f^{(s)}(0) - F_\sigma^{(s)}(0) \right| + \left| F_\sigma^{(s)}(0) - D^{[s]}_{h,N}[F_\sigma] \right| + \left| D^{[s]}_{h,N}[f - F_\sigma] \right|.
\]

(44)

Now we choose \( \sigma := \pi/(4h) \) and estimate the three terms on the right-hand side.

Under the hypotheses on \( f \), it is known [32, p. 260, §5.1.4] that

\[
\| f - F_\sigma \|_\infty = O \left( \sigma^{-m-\kappa} \right) \quad (\sigma \to +\infty),
\]

or equivalently,

\[
\| f - F_\sigma \|_\infty = O \left( h^{m+\kappa} \right) \quad (h \to 0_+).
\]

(45)

Using this, we infer from a result of Junggeburth, Scherer and Trebels (see the implication (i) \( \Rightarrow \) (ii) in [18, Satz 5a]) that

\[
\left| f^{(s)}(0) - F_\sigma^{(s)}(0) \right| = O \left( h^{m+\kappa-s} \right) \quad (h \to 0_+).
\]

(46)

For estimating the second term on the right-hand side of (44), we employ Theorem 2 with \( z = \pi/4 \). It implies that

\[
\left| F_\sigma^{(s)}(0) - D^{[s]}_{h,N}[F_\sigma] \right| \leq \frac{2s!e^{-\pi N/4}}{\pi N^m s! h^s} \| F_\sigma \|_\infty,
\]

where \( m_s = 3/2 \) for odd \( s \) and \( m_s = 5/2 \) for even \( s \). Since \( 0 \in B^\infty_\sigma \), we obviously have \( \| F_\sigma \|_\infty \lesssim 2\| f \|_\infty \). Furthermore, the choice of \( N \) implies that

\[
e^{-\pi N/4} \lesssim e^{\pi/4} h^{m+\kappa}.
\]

Hence

\[
\left| F_\sigma^{(s)}(0) - D^{[s]}_{h,N}[F_\sigma] \right| = o \left( h^{m+\kappa-s} \right) \quad (h \to 0_+).
\]

(47)

Next we note that the functional \( D^{[s]}_{h,N} \) applies to every function \( g \in C_B(\mathbb{R}) \) and, by a crude estimate not distinguishing between odd and even \( s \), we have

\[
\left| D^{[s]}_{h,N}[g] \right| \leq 4s! \sum_{n=-\infty}^{\infty} \left| P_{\left(s+1/2\right)} \left( \frac{\pi}{16N}; \frac{1}{(2n - 1)^2} \right) \right| \cdot \| g \|_\infty.
\]
A discussion of the coefficients of the polynomial \( P_{\lfloor (s+1)/2 \rfloor} \) as in the proof of Theorem 2 shows the existence of a constant \( K_s \), depending on \( s \) only, such that
\[
\left| D_{h,N}^{[s]} [g] \right| \leq \frac{K_s}{h^s} \|g\|_{\infty}.
\]
Using this estimate for \( g := f - F_\sigma \) and recalling (45), we obtain
\[
\left| D_{h,N}^{[s]} [f - F_\sigma] \right| = O \left( h^{m+\kappa-s} \right) \quad (h \to 0_+).
\] (48)

The proof is completed by combining (44) and (46)–(48).

We add four remarks.

**Remark 9.** The paper [18] is not easily available, it is not in English, and it is not easy to read since it cares for a high degree of generality and needs a sophisticated notation. For these reasons, we mention that in the proof of Theorem 8, we could alternatively follow Timan [32, pp. 258–259] who constructs a function \( Q_\sigma(f; \cdot) \in B_\alpha^\infty \) which achieves the order of best approximation to \( f \) and, as is easily seen from the special form of this function, \( Q_\sigma^{(s)}(f; \cdot) \) achieves the order of best approximation to \( f^{(s)} \). The preceding proof remains valid with \( F_\sigma \) replaced by \( Q_\sigma(f; \cdot) \). However, it is a gain to absorb the material in [18].

**Remark 10.** Under the same hypotheses on \( f \), the rate of convergence in [7, Theorem] is the same as in Theorem 8. However, while in [7] the approximation is by a series, it is here by a finite sum with the number of terms proportional to \( \log(1/h) \) only.

**Remark 11.** The method of Theorem 8 has some features of a finite difference method with a restricted number of nodes. In order to increase the accuracy, we have to decrease \( h \). In doing so, the number of nodes increases, but it increases slowly. All the nodes approach zero and so does \( d^* \). For small \( h > 0 \), there may be danger of subtractive cancellation.

**Remark 12.** If the assumptions concerning the regularity of \( f \) hold on a finite interval \([-a, a]\) only, it is still justified to use the formulae of Theorem 8. Indeed, for sufficiently small \( h > 0 \), all the nodes will lie in a subinterval of \([-a, a]\), and we may think of restricting \( f \) to this subinterval and continuing the restriction to the whole of \( \mathbb{R} \) such that it satisfies the hypotheses of Theorem 8.

5. Examples

**Example 13.** Let \( f(x) := \sin(x + \pi/4) \). Then (11) holds with \( \sigma = 1 \) and \( \phi(x) \equiv 1 \). We want to use the formulae of Theorem 2 (or Lemma 1) for approximating \( f'(0) \) and \( f''(0) \); see (7) and (8) with \( \omega := (\pi - 2h)/(8N) \). In particular, we are interested in comparing the error bounds deducible from (13) with the true errors and in comparing the true errors with those of the corresponding formulae in [24] or [25, for \( b = 1 \)]. For similarly spaced nodes, the latter take the form
\[
f'(0) = \frac{1}{2h} \sum_{n=1}^{N} \frac{(-1)^n + 1}{n} e^{-\omega(2n)^2} \left[ f(2nh) - f(-2nh) \right] + \text{remainder}
\] (49)
Table 1
Approximation of derivatives of \( f(x) := \sin(x + \frac{\pi}{4}) \) at \( x = 0 \).

<table>
<thead>
<tr>
<th>( \sigma = 1 )</th>
<th>Absolute error of ( f'(0) )</th>
<th>Absolute error of ( f''(0) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h = \frac{1}{4} )</td>
<td>Theorem 2 (49)</td>
<td>Theorem 2 (50)</td>
</tr>
<tr>
<td>( N )</td>
<td>Bound</td>
<td>True value</td>
</tr>
<tr>
<td>2</td>
<td>8.38E-02</td>
<td>1.35E-02</td>
</tr>
<tr>
<td>4</td>
<td>1.86E-03</td>
<td>3.93E-04</td>
</tr>
<tr>
<td>8</td>
<td>3.01E-06</td>
<td>6.28E-07</td>
</tr>
<tr>
<td>16</td>
<td>2.54E-11</td>
<td>7.25E-12</td>
</tr>
<tr>
<td>32</td>
<td>5.61E-21</td>
<td>1.59E-21</td>
</tr>
</tbody>
</table>

and

\[
f''(0) = \frac{1}{2h^2} \sum_{n=1}^{N} (-1)^{n+1} \left( 8\omega + \frac{1}{n^2} \right) e^{-\omega(2n)^2} \left[ f(2nh) - 2f(0) + f(-2nh) \right] + \text{remainder}
\]

(50)

with the same \( \omega \) as specified before. In [24,25], bounds for the remainders were obtained for \( f \in B_{\sigma}^2 \) only.

The results for \( h = 1/4 \) are given in Table 1. It is remarkable that the error bounds are quite realistic, that is, they do not overestimate the true errors very much. The formulae of Theorem 2 are more precise than (49) and (50). The improvement is by a factor of about \( 1/(3.5N) \) in case of the first derivative and \( 1/(7.7N^2) \) in case of the second derivative. Experiments have shown that varying \( h \) around \( 1/4 \) has no drastic influence on the errors. As expected by the theory, increasing \( N \) is much more effective than diminishing \( h \).

**Example 14.** The function \( f : z \mapsto z/(4 + z^2) \) is analytic and bounded on each square \( Q_d \) for \( 0 < d < 2 \). Therefore Theorem 6 applies. Alternatively, we may consider the mapping

\[
\psi : z \mapsto 2d \frac{\log \left( \frac{1 - z}{1 + z} \right)}{\pi}.
\]

For \( d \in (0, 2) \), it maps \( Q_1 \) onto an unbounded domain \( S_d \), say, on which \( f \) is also analytic and bounded. We note that \( \{ z \in \mathbb{C} : |z| \leq d \} \subset S_d \), and so \( Q_d \subset S_d \). Furthermore, \( \psi(0) = 0 \). In view of Remark 7, we may therefore apply Theorem 6 to \( f \circ \psi \). For the first derivative, we arrive at the formula

\[
f'(0) = -\frac{1}{2hd} \sum_{n=1}^{N} (-1)^{n+1} \frac{(2n-1)^2}{(2n-1)^2} e^{-\omega(2n-1)^2} \delta_n(f \circ \psi)_h + \text{remainder},
\]

(51)

where \( h = 1/(2N) \) and \( \omega = \pi/(8N) \). Since this formula makes use of the fact that \( f \) is analytic and bounded not only on \( Q_d \) but on the larger domain \( S_d \), we may hope that it is more accurate.

Numerical experiments show that the choice of \( d \) does not have much influence on the accuracy as long as \( d \) is not too close to 2. Table 2 shows the results for \( d = 1 \) and 9/5. For
Table 2
Approximation of the derivative of a function with poles.

<table>
<thead>
<tr>
<th>$d = 1$</th>
<th>Absolute error of $f'(0)$</th>
<th>$d = \frac{9}{5}$</th>
<th>Absolute error of $f''(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>Theorem 6 (51)</td>
<td>$N$</td>
<td>Theorem 6 (51)</td>
</tr>
<tr>
<td>2</td>
<td>8.35E−03</td>
<td>2</td>
<td>1.35E−02</td>
</tr>
<tr>
<td></td>
<td>6.65E−03</td>
<td>4</td>
<td>5.03E−04</td>
</tr>
<tr>
<td>8</td>
<td>3.65E−07</td>
<td>8</td>
<td>7.97E−07</td>
</tr>
<tr>
<td>16</td>
<td>9.12E−13</td>
<td>16</td>
<td>2.31E−12</td>
</tr>
<tr>
<td>32</td>
<td>7.88E−24</td>
<td>32</td>
<td>2.28E−23</td>
</tr>
</tbody>
</table>

$d = 1$, formula (51) is always slightly better than the formula of Theorem 6, but we would have expected a more significant improvement.

Example 15. Let

$$f(x) := \sin(3x) + \frac{(3x)_7}{7!} \quad \text{and} \quad g(x) := \cos(3x) - \frac{(3x)_8}{8!},$$

where $x_+ := (|x| + x)/2$. Note that $f(x) = \sin(3x)$ for negative $x$ while for positive $x$ we obtain $f(x)$ by taking the power series of $\sin(3x)$ and deleting the term containing $x^7$. A corresponding observation holds for $g$. These functions do not satisfy all the hypotheses of Theorem 8 since they are not bounded on $\mathbb{R}$. However, in view of Remark 12, we may apply the formulae of Theorem 8 with $a = 1$ and $m = 6$ in the case of $f$ and $m = 7$ in the case of $g$. Hence

$$f'(0) - D_{h,N}^{[1]}[f] = O(h^6) \quad \text{and} \quad g''(0) - D_{h,N}^{[2]}[g] = O(h^6) \quad (h \to 0_+).$$

We also consider two familiar finite difference formulae, namely

$$f'(0) = \frac{f(-2h) - 8f(-h) + 8f(h) - f(2h)}{12h} + \frac{h^4}{30} f^{(5)}(\xi) \quad (-2h \leq \xi \leq 2h)$$

and

$$g''(0) = \frac{-g(-2h) + 16g(-h) - 30g(0) + 16g(h) - g(2h)}{12h^2} + \frac{h^4}{90} f^{(7)}(\xi) \quad (-2h \leq \xi \leq 2h).$$

For the truncated powers in (52), these formula also have a remainder of order $O(h^6)$ but the trigonometric terms reduce the order to $O(h^4)$. On the other hand, the truncated powers restrict the order of convergence of the formulae of Theorem 8. In the absence of the truncated powers, Theorem 2 would apply yielding exponential convergence.

Numerical results are shown in Table 3. For $k = 4, 8, 16, \ldots$, we have chosen $h = 1/k$. Then the formulae of Theorem 8 require $N = \lfloor (28/\pi) \log k \rfloor$ for $f$ and $N = \lfloor (32/\pi) \log k \rfloor$ for $g$. Thus, other than in the finite difference formulae, the number of nodes increases with decreasing $h$ but the accuracy is higher. In view of stability, we should also look at the minimal span $2h$ of the arguments of the involved differences of function values. For achieving an accuracy of about seven
Table 3
Approximation of derivatives of non-analytic functions.

<table>
<thead>
<tr>
<th>$h = \frac{1}{k}$</th>
<th>$N$</th>
<th>Absolute error of $f'(0)$</th>
<th>$h = \frac{1}{k}$</th>
<th>$N$</th>
<th>Absolute error of $g''(0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$kN$</td>
<td>Theorem 8</td>
<td>$(53)$</td>
<td>$kN$</td>
<td>Theorem 8</td>
<td>$(54)$</td>
</tr>
<tr>
<td>4</td>
<td>12</td>
<td>1.87E−02</td>
<td>3.06E−02</td>
<td>4</td>
<td>14</td>
</tr>
<tr>
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<td>18</td>
<td>1.96E−03</td>
<td>1.97E−03</td>
<td>8</td>
<td>21</td>
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<tr>
<td>16</td>
<td>24</td>
<td>1.06E−04</td>
<td>1.23E−04</td>
<td>16</td>
<td>28</td>
</tr>
<tr>
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<td>30</td>
<td>4.53E−12</td>
<td>7.72E−06</td>
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<td>35</td>
</tr>
<tr>
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<td>3.78E−16</td>
<td>4.83E−07</td>
<td>64</td>
<td>42</td>
</tr>
<tr>
<td>128</td>
<td>43</td>
<td>1.61E−17</td>
<td>3.02E−08</td>
<td>128</td>
<td>49</td>
</tr>
</tbody>
</table>

correct decimal places, the formulae of Theorem 8 need a minimal span lying between 0.125 and 0.25 while the finite difference formulae need about 0.015625.

References