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Higher order pseudospectral differentiation matrices

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Abstract

A new explicit expression of the higher order pseudospectral differentiation matrices is presented by using an explicit formula for higher derivatives of Chebyshev polynomials. The roundoff errors incurred during computing differentiation matrices are investigated. The advantages of the suggested differentiation matrices emerged through comparisons with other ones.

Keywords: Chebyshev collocation; Differentiation matrix; Roundoff error; Chebyshev polynomials

1. Introduction

The concept of a differentiation matrix is developed in the last two decades and it has proven to be a very useful tool in the numerical solution of differential equations [9,14]. Differentiation matrices are derived from the spectral collocation method for solving differential equations of boundary value type. Spectral collocation methods, also known as pseudospectral methods, are obtained when the test functions in the variational formulation are Dirac functions based on a pre-determined set of collocation points. The resulting scheme approximates the derivatives by differentiating a global interpolant built

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through the collocation points. For the explicit expressions of the entries of the differentiation matrices and further details of collocation methods, we refer to [7,9,14,19].

The set of collocation points is related to the set of basis functions as the nodes of quadrature formulae, which are used in the computation of the spectral coefficients from the grid values. For nonperiodic problems, Chebyshev polynomials are usually taken with their associated collocation points in the interval $[-1,1]$ given by

$$x_k = \cos\frac{k\pi}{N}, \quad k = 0, 1, \dots, N. \tag{1}$$

An explicit expression of $\overline{D}$ using the Chebyshev–Lobatto points is given by [9]

$$\overline{D}_{ij} = \begin{cases} \frac{2N^2+1}{6} & i = j = 0, \\ -\frac{2N^2+1}{6} & i = j = N, \\ -\frac{x_j}{2(1-x_j^2)} & i = j \neq 0, N, \\ \frac{\gamma_i}{\gamma_j}\frac{(-1)^{(i+j)}}{x_i - x_j} & i \neq j, \end{cases} \tag{2}$$

where $\gamma_j = 1$, except for $\gamma_0 = \gamma_N = 2$.

To get the higher orders of derivative matrices we can use explicit expressions or just $\overline{D}^{(p)} = (\overline{D})^p$, which does not work for every set of collocation points [3]. The matrix product $\overline{D}\underline{f}$ is the Chebyshev pseudospectral approximation to $\underline{f}'$ where $\underline{f} = [f(x_0), f(x_1), \dots, f(x_N)]^{\mathrm{T}}$ and $\underline{f}' = [f'(x_0), f'(x_1), \dots, f'(x_N)]^{\mathrm{T}}$. If it is computed by matrix$-$vector multiplication, then the total number of operations is $2N^2$, while, this matrix product can be computed in N^2 operations by using Solomonoff's algorithm [17]. It is important to remark that for large N the direct implementation of (2) suffers from cancellation, causing large errors in the elements of the matrix $\overline{D}$ [5,18]. For example, in [1,8] it is shown that the absolute error in the evaluation of $\overline{D}_{01}$ is of order $\mathrm{O}(N^4\varepsilon)$, where ε is the machine precision, giving an overall error of order $\mathrm{O}(N^4\varepsilon)$ in the evaluation of the first derivative near the boundary. A modification of the differentiation matrix (2) is presented in [18] by Tang and Trummer, where the evaluations of the elements of the matrix (2) are done by means of their trigonometric expressions and this replaces (2) by

$$\overline{D}_{ij} = \begin{cases} -\frac{x_i}{2\sin^2(\frac{i\pi}{N})} & i = j \neq 0, N, \\ -\frac{\gamma_i}{2\gamma_j}\frac{(-1)^{(i+j)}}{\sin(\frac{(i+j)\pi}{2N})\sin(\frac{(i-j)\pi}{2N})} & i \neq j, \end{cases} \tag{3}$$

with γ_j as before and without modifying in Eq. (2) for $i = j = 0$ and $i = j = N$. This modification leads to a gain of a few digits of precision [3,4].

Another way of computing the differentiation matrices utilizes (2) for the off-diagonal entries but then obtains the diagonal entries from "the negative sum trick" [1]

$$\overline{D}_{ii} = -\sum_{\substack{k=0 \\ k\neq i}}^{N} \overline{D}_{ik}.$$

Therefore [16],

$$\overline{D}_{ij} = \begin{cases} \frac{\gamma_i}{\gamma_j} \frac{(-1)^{i+j}}{x_i - x_j} & i \neq j, \\ -\sum_{\substack{k=0 \\ k\neq i}}^{N} \overline{D}_{ik} & i = j. \end{cases} \tag{4}$$

Baltensperger [2] presents a formula

$$\gamma_k = \prod_{\substack{i=0 \\ i\neq k}}^{N} \frac{1}{x_k - x_i},$$

for extending the algorithm (4) to any set of collocation points.

In [13], Don and Solomonoff showed how to compute higher derivatives for the Chebyshev collocation method. They depend on transforming the collocation points to new ones. Welfert [20] present a recursive formula for evaluating the higher derivatives at various types of collocation points. Costa and Don [10] present efficient and accurate recursive algorithms for evaluating the entries of the differentiation matrices for higher derivatives using the well-known Lagrangian interpolation formulation.

In this paper, we present a simple formula to evaluate the ith derivative of the Chebyshev polynomials. Also, we show how to construct the Chebyshev collocation derivatives by constructing the entries of the differentiation matrices. We discuss the roundoff errors resulting during computing the entries of the first four differentiation matrices.

The analysis and the results presented in this paper are valid only for the case of Chebyshev extrema nodes $x_k = \cos\frac{k\pi}{N},\ k = 0, 1, \ldots, N$.

2. Higher derivatives of Chebyshev polynomials

Let $f(x)$ be a smooth function given by a Chebyshev series

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x), \tag{5}$$

where

$$T_n(x) = \cos\bigl(n \cos^{-1} x\bigr).$$

Then the ith derivative of $f(x)$ has a series expansion of the form

$$f^{(i)}(x) = \sum_{n=0}^{\infty} a_n^{(i)} T_n(x). \tag{6}$$

A relation between the coefficients $a_n^{(i)}$ and a_n is given by Doha [11],

$$c_n a_n^{(i)} = \frac{2^i}{(i-1)!} \sum_{k=1}^{\infty} \frac{(k+i-2)!(n+k+i-2)!(n+2k+i-2)}{(k-1)!(n+k-1)!} a_{n+2k+i-2}, \tag{7}$$

where $c_0 = 2,\ c_i = 1,\ i \geqslant 1$.

The following theorem has fundamental importance in developing the present work.

Theorem 1. *The derivatives of the Chebyshev polynomials are given by*

$$T_k^{(i)}(x) = \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} b_{n,k}^i T_n(x), \quad k \geqslant i, \tag{8}$$

with

$$b_{n,k}^i = \frac{2^i k}{(i-1)!c_n} \frac{(s-n+i-1)!(s+i-1)!}{(s)!(s-n)!}, \tag{9}$$

where $2s = k + n - i$.

Proof. The ith derivative of Eq. (5) gives

$$f^{(i)}(x) = \sum_{l=i}^{\infty} a_l T_l^{(i)}(x). \tag{10}$$

Substitution of Eq. (7) into Eq. (6) gives

$$f^{(i)}(x) = \sum_{n=0}^{\infty} \frac{2^i}{(i-1)!c_n} \sum_{k=1}^{\infty} \frac{(k+i-2)!(n+k+i-2)!(n+2k+i-2)}{(k-1)!(n+k-1)!} a_{n+2k+i-2} T_n(x).$$

Set an integer $l = n + 2k + i - 2$ and $2m = l + n - i$, we get

$$f^{(i)}(x) = \sum_{n=0}^{\infty} \frac{2^i}{(i-1)!c_n} \sum_{\substack{l=n+i \\ (l+n-i)\ \text{even}}}^{\infty} g_{n,l}^i T_n(x), \tag{11}$$

where

$$g_{n,l}^i = \frac{(m-n+i-1)!(m+i-1)!}{(m)!(m-n)!} l a_l.$$

We note that

$$\frac{2^i g_{n,k}^i}{(i-1)!c_n} = b_{n,k}^i a_k.$$

In view of Eq. (10), Eq.(11) becomes

$$\sum_{n=0}^{\infty} \sum_{\substack{l=n+i \\ (l+n-i)\ \text{even}}}^{\infty} b_{n,l}^i a_l T_n(x) = \sum_{l=i}^{\infty} a_l T_l^{(i)}(x).$$

Equating the coefficients of a_k, $k \geqslant i$, gives Eqs. (8) and (9). By doing so, the proof is completed. □

3. Chebyshev differentiation matrices

We approximate the derivatives of a function $f(x)$ by interpolating the function with a polynomial at the Chebyshev extrema nodes x_k, differentiating the polynomial, and then evaluating the polynomial at the same nodes. With $f_k = f(x_k)$ we construct a global Nth order Chebyshev interpolating polynomial

$$(P_N f)(x) = \sum_{j=0}^{N} f_j \varphi_j(x), \tag{12}$$

to obtain the approximation of the function $f(x)$, where

$$\varphi_j(x) = \frac{2\theta_j}{N} \sum_{k=0}^{N} \theta_k T_k(x_j) T_k(x),$$

$$\varphi_j(x_k) = \begin{cases} 0 & j \neq k, \\ 1 & j = k, \end{cases}$$

and $\theta_j = 1$, except for $\theta_0 = \theta_N = \frac{1}{2}$. The projection operator $(P_N f)(x)$ is a unique Nth degree interpolating polynomial such that

$$(P_N f)(x_j) = f(x_j), \quad j = 0, 1, \ldots, N.$$

Alternatively, the interpolating polynomial $(P_N f)(x)$ can be expressed in terms of series expansion of the classical Chebyshev polynomials

$$(P_N f)(x) = \sum_{n=0}^{N} a_n T_n(x),$$

where

$$a_n = \frac{2\theta_n}{N} \sum_{j=0}^{N} \theta_j f_j T_n(x_j).$$

We use the Chebyshev extrema nodes $x_k = \cos\frac{k\pi}{N}$, $k = 0(1)N$, as interpolated points. The derivatives of $f(x)$ can be estimated at the points x_k by differentiating Eq. (12) and evaluating the resulting expression. This yields

$$(P_N f)^{(i)}(x) = \sum_{j=0}^{N} f_j \varphi_j^{(i)}(x).$$

Using Theorem 1, the ith derivative of the interpolating polynomial $(P_N f)(x)$ is given by

$$(P_N f)^{(i)}(x) = \sum_{j=0}^{N} \frac{2}{N} f_j \theta_j \sum_{k=i}^{N} \theta_k T_k(x_j) \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} b_{n,k}^{i} T_n(x).$$

Setting $\underline{f} = [f(x_0), f(x_1), \ldots, f(x_N)]^{\mathrm{T}}$ and $\underline{f}^{(i)} = [f^{(i)}(x_0), f^{(i)}(x_1), \ldots, f^{(i)}(x_N)]^{\mathrm{T}}$. We approximate the derivatives of $f(x)$ at the points x_j, $j = 0, 1, \ldots, N$, by the equation

$$\underline{f}^{(i)} = D^{(i)} \underline{f}.$$

The entries of the matrix $D^{(i)}$ are given by

$$d^i_{l,j} = \frac{2\theta_j}{N} \sum_{k=i}^{N} \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} \theta_k b^i_{n,k} T_k(x_j) T_n(x_l). \tag{13}$$

We now present two different ways of alleviating errors. The first way is to use trigonometric identities and replace (13) by the formula

$$d^i_{l,j} = \frac{2\theta_j}{N} \sum_{k=i}^{N} \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} \theta_k b^i_{n,k} \cos\frac{kj\pi}{N} \cos\frac{nl\pi}{N}. \tag{14}$$

The second way is based on the use of periodic properties of the cosine function and replace (14) by the formula

$$d^i_{l,j} = \frac{2\theta_j}{N} \sum_{k=i}^{N} \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} \theta_k b^i_{n,k} (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} x_{kj-N[\frac{kj}{N}]} x_{nl-N[\frac{nl}{N}]}, \tag{15}$$

or

$$d^i_{l,j} = \frac{\theta_j}{N} \sum_{k=i}^{N} \sum_{\substack{n=0 \\ (n+k-i)\ \text{even}}}^{k-i} \theta_k b^i_{n,k} \Big((-1)^{[\frac{kj+nl}{N}]} x_{(kj+nl)-[\frac{kj+nl}{N}]N} + (-1)^{[\frac{kj-nl}{N}]} x_{(kj-nl)-[\frac{kj-nl}{N}]N}\Big). \tag{16}$$

The improvement of the results can be seen in Tables 2–9. The elements $d^i_{l,j}$ satisfy anticentrosymmetry property.

$$d^i_{l,j} = -d^i_{N-l,N-j}, \quad l, j = 0, 1, \ldots, N.$$

In the next section we focus on the first four derivatives from Eq. (15) which can be rewritten in the following simple forms

$$d^1_{l,j} = \frac{4\theta_j}{N} \sum_{k=1}^{N} \sum_{\substack{n=0 \\ (n+k)\ \text{odd}}}^{k-1} \frac{\theta_k k}{c_n} (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} x_{kj-N[\frac{kj}{N}]} x_{nl-N[\frac{nl}{N}]}, \tag{17}$$

$$d^2_{l,j} = \frac{2\theta_j}{N} \sum_{k=2}^{N} \sum_{\substack{n=0 \\ (n+k)\ \text{even}}}^{k-2} \frac{k\theta_k pq}{c_n} (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} x_{kj-N[\frac{kj}{N}]} x_{nl-N[\frac{nl}{N}]}, \tag{18}$$

$$d^3_{l,j} = \frac{\theta_j}{N} \sum_{k=3}^{N} \sum_{\substack{n=0 \\ (n+k)\ \text{odd}}}^{k-3} \frac{\theta_k k}{2c_n} \big(p^2-1\big)\big(q^2-1\big) (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} x_{kj-N[\frac{kj}{N}]} x_{nl-N[\frac{nl}{N}]}, \tag{19}$$

and

$$d^4_{l,j} = \frac{\theta_j}{N} \sum_{k=4}^{N} \sum_{\substack{n=0 \\ (n+k)\ \text{even}}}^{k-4} \frac{\theta_k kpq}{12c_n} \big(p^2-4\big)\big(q^2-4\big) (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} x_{kj-N[\frac{kj}{N}]} x_{nl-N[\frac{nl}{N}]}, \tag{20}$$

where $p = k - n$ and $q = k + n$.

4. Rounding error analysis

We investigate the effect of roundoff error on the elements $d^i_{l,j}$ in Eqs. (17)–(20). In finite precision arithmetic, however, we have

$$x_k^* = x_k + \delta_k,$$

where δ_k denotes a small error, with $|\delta_k|$ approximately equal to machine precision ε and $\delta = \max_k\{|\delta_k|\}$; we use the notation x_k^* for the exact value whereas x_k for the computed value. The absolute errors of the quantities $x_k x_n$ still being on the order of machine precision.

$$\left|x_k^* x_n^* - x_k x_n\right| = (\delta_k + \delta_n) - \mathrm{O}\left(\frac{1}{N^2}\delta_k\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_n\right).$$

4.1. Error bound for the first order derivatives

By using Eq. (17) to evaluate the elements of the first order differentiation matrix, there would be roundoff error as in:

$$\begin{aligned}
d^{1*}_{l,j} - d^1_{l,j} &= \frac{2\theta_j}{N}\sum_{k=1}^{N}\sum_{\substack{n=0\\(n+k)\ \text{odd}}}^{k-1}\theta_k\frac{2k}{c_n}(-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]}\\
&\quad\times\left((\delta_{kj-N[\frac{kj}{N}]}+\delta_{nl-N[\frac{nl}{N}]}) - \mathrm{O}\left(\frac{1}{N^2}\delta_{kj-N[\frac{kj}{N}]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{nl-N[\frac{nl}{N}]}\right)\right)\\
&\leqslant \frac{4\theta_j}{N}\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\sum_{k=1}^{N}\theta_k k^2\\
&\leqslant 4\theta_j\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\left(\frac{N^2}{3}+\frac{1}{6}\right).
\end{aligned}$$

The element d^1_{01} is the major elements concerning its values. Accordingly, it bears the major error responsibility comparing the other elements. In [1], Baltensperger and Trummer show that the error in the evaluation of the element $\overline{D}_{01}$ from the classical matrix (2) is of order $\mathrm{O}(N^4\delta)$ where

$$\overline{D}^*_{01} - \overline{D}_{01} = \frac{8N^4}{\pi^4}\delta,$$

whereas we find the error in d^1_{01} is of order $\mathrm{O}(N^2\delta)$. This can be taken into consideration, as itself, as modifying for the classical matrix (2). We have

$$d^1_{01} = \frac{2}{N}\sum_{k=1}^{N-1}k^2 x_k - N = -\frac{1}{3} + \left(-\frac{4}{\pi^2}\right)N^2 + \mathrm{O}\left(\frac{1}{N^2}\right),$$

with error upper bound

$$d^{1*}_{01} - d^1_{01} = \frac{2}{N}\sum_{k=1}^{N-1}k^2\delta_k \leqslant \left(\frac{1}{3} - N + \frac{2}{3}N^2\right)\delta.$$

Table 1
Computed errors in d^1_{01} and $\overline{D}_{01}$

N	$d^{1*}_{01} - d^1_{01}$	Error upper bound $(\frac{1}{3} - N + \frac{2}{3}N^2)\delta$	$\overline{D}^*_{01} - \overline{D}_{01}$
16	7.80×10^{-15}	3.44×10^{-14}	9.78×10^{-14}
32	4.06×10^{-14}	1.45×10^{-13}	3.64×10^{-12}
64	9.07×10^{-14}	5.92×10^{-13}	1.70×10^{-11}
128	3.05×10^{-13}	2.40×10^{-12}	6.58×10^{-10}
256	5.29×10^{-12}	9.64×10^{-12}	1.34×10^{-08}
512	2.15×10^{-12}	3.87×10^{-11}	1.89×10^{-07}
1024	9.35×10^{-12}	1.55×10^{-10}	1.78×10^{-06}
2048	3.88×10^{-10}	6.20×10^{-10}	4.43×10^{-05}
4096	2.39×10^{-09}	2.48×10^{-09}	1.73×10^{-04}

Table 1 lists the computed errors in the elements d^1_{01} and $\overline{D}_{01}$. The exact values was computed with 25 digit precision using MATHEMATICA™.

In view of Eqs. (16) and (17), the elements of the first and last rows of the differentiation matrix $D^{(1)}$ are computed from the simple form

$$d^1_{0j} = \frac{2\theta_j}{N}\sum_{k=1}^{N-1}(-1)^{[\frac{kj}{N}]}k^2 x_{kj-N[\frac{kj}{N}]} + (-1)^j\theta_j N,$$

with error upper bound

$$d^{1*}_{0j} - d^1_{0j} = \frac{2\theta_j}{N}\sum_{k=1}^{N-1}(-1)^{[\frac{kj}{N}]}k^2\delta_{kj-N[\frac{kj}{N}]} \leqslant \frac{2\theta_j\delta}{N}\left(\sum_{k=1}^{N-1}(-1)^{[\frac{kj}{N}]}k^2\right) \leqslant \left(\frac{1}{3} - N + \frac{2}{3}N^2\right)\delta.$$

The error bounds for the higher derivatives are clear extensions of the result in Section 4.1 and this will be pointed out in Appendix A.

5. Accuracy in computing higher derivatives

Several authors have presented different ideas for alleviating the effects of roundoff errors in the calculation of derivatives and differentiation matrices for collocation points. In [8], the authors alleviate the error by preconditioning the problem. Don and Solomonoff in [12], and Tang and Trummer in [18], use trigonometric identities and a flipping trick to alleviate rounding errors. In [15], the authors propose a coordinate transform resulting in better stability property. Also, negative sum trick approach is suggested by [3,4,6]. In this approach the diagonal of the matrix is modified to satisfy a relation among the entries of the differentiation matrix. This relation is the row sums of a spectral differentiation matrix are all equal to zero.

We believe that these ideas can be used to improve the accuracy for the suggested matrices. That will be shown in further research work.

In this section we present the result of two numerical tests done in double precision with unit round off $\varepsilon = 2.22 \times 10^{-16}$. All the tests have been performed on a PC-Pentium III and the programs have been written in Fortran 90.

We now show some numerical experiments due to formulae (2)–(4), (14)–(16). We compute the first four derivatives of the test functions $f(x) = x^8$ and $f(x) = \sin x$. When looking at the function $f(x) = x^8$ all the errors observed are due to roundoff, hence we have increasing errors with N [1]. The ith derivative is computed by multiplying the vector $\underline{f} = [f(x_0), f(x_1), \ldots, f(x_N)]^{\mathrm{T}}$ by the derivatives matrix $D^{(i)}$. Tables 2–9 shows the maximum absolute error for the first four derivatives of the functions $f(x) = x^8$ and $f(x) = \sin x$ for different numbers of Chebyshev collocation points.

Table 2
The maximum absolute error for the first derivative of $f(x) = x^8$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	1.7×10^{-13}	1.4×10^{-14}	1.2×10^{-14}	8.7×10^{-14}	1.7×10^{-13}	1.2×10^{-14}
32	9.3×10^{-13}	1.9×10^{-13}	2.3×10^{-13}	5.7×10^{-12}	3.5×10^{-13}	1.1×10^{-13}
64	4.2×10^{-12}	3.6×10^{-13}	9.1×10^{-13}	2.3×10^{-11}	2.7×10^{-12}	3.8×10^{-13}
128	4.2×10^{-11}	2.4×10^{-12}	1.0×10^{-11}	6.4×10^{-10}	3.9×10^{-11}	2.1×10^{-12}
256	4.2×10^{-10}	1.5×10^{-11}	1.8×10^{-11}	1.4×10^{-08}	1.4×10^{-09}	2.1×10^{-11}
512	3.8×10^{-09}	2.9×10^{-11}	2.7×10^{-10}	1.8×10^{-07}	1.7×10^{-09}	2.2×10^{-11}

Table 3
The maximum absolute error for the second derivative of $f(x) = x^8$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	5.2×10^{-12}	9.1×10^{-13}	7.8×10^{-13}	1.1×10^{-11}	1.8×10^{-11}	1.3×10^{-12}
32	2.0×10^{-10}	5.1×10^{-11}	5.1×10^{-11}	2.5×10^{-09}	1.0×10^{-10}	3.4×10^{-11}
64	4.1×10^{-09}	1.4×10^{-10}	1.3×10^{-10}	5.1×10^{-08}	3.7×10^{-09}	4.9×10^{-10}
128	1.9×10^{-07}	1.1×10^{-08}	1.1×10^{-08}	4.7×10^{-06}	2.7×10^{-07}	1.2×10^{-08}
256	7.0×10^{-06}	2.6×10^{-07}	2.6×10^{-07}	4.1×10^{-04}	3.6×10^{-05}	1.2×10^{-06}
512	2.6×10^{-04}	6.2×10^{-06}	1.1×10^{-05}	1.8×10^{-02}	3.7×10^{-05}	2.5×10^{-05}

Table 4
The maximum absolute error for the third derivative of $f(x) = x^8$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	4.6×10^{-10}	2.2×10^{-11}	2.2×10^{-11}	4.9×10^{-10}	4.5×10^{-11}	2.2×10^{-10}
32	3.4×10^{-08}	7.6×10^{-09}	7.6×10^{-09}	5.6×10^{-07}	5.6×10^{-08}	4.5×10^{-09}
64	3.4×10^{-06}	8.3×10^{-07}	8.3×10^{-07}	5.1×10^{-05}	4.3×10^{-07}	1.8×10^{-07}
128	4.0×10^{-04}	1.9×10^{-05}	1.7×10^{-05}	1.7×10^{-02}	1.3×10^{-04}	1.4×10^{-04}
256	1.9×10^{-02}	2.2×10^{-03}	2.5×10^{-03}	5.9×10^{-00}	1.8×10^{-02}	3.4×10^{-03}
512	1.0×10^{-01}	8.2×10^{-01}	1.4×10^{-01}	$9.8 \times 10^{+02}$	$1.8 \times 10^{+01}$	1.1×10^{-00}

Table 5
The maximum absolute error for the fourth derivative of $f(x) = x^8$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	6.8×10^{-09}	9.4×10^{-10}	1.1×10^{-09}	2.2×10^{-08}	4.3×10^{-08}	2.8×10^{-09}
32	4.5×10^{-06}	1.2×10^{-06}	1.2×10^{-06}	8.7×10^{-05}	5.3×10^{-07}	1.2×10^{-06}
64	1.7×10^{-03}	4.3×10^{-04}	4.3×10^{-04}	3.3×10^{-02}	1.4×10^{-03}	8.3×10^{-04}
128	8.1×10^{-01}	3.1×10^{-02}	4.9×10^{-02}	$4.1 \times 10^{+01}$	$2.2 \times 10^{+00}$	1.5×10^{-01}
256	$6.7 \times 10^{+02}$	$1.9 \times 10^{+01}$	$1.9 \times 10^{+01}$	$5.8 \times 10^{+04}$	$4.8 \times 10^{+03}$	$6.9 \times 10^{+01}$
512	$3.2 \times 10^{+05}$	$8.8 \times 10^{+03}$	$4.2 \times 10^{+03}$	$3.8 \times 10^{+07}$	$9.0 \times 10^{+03}$	$1.4 \times 10^{+04}$

Table 6
The maximum absolute error for the first derivative of $f(x) = \sin x$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	1.2×10^{-13}	4.3×10^{-15}	1.3×10^{-14}	8.7×10^{-14}	1.5×10^{-13}	1.3×10^{-14}
32	1.4×10^{-12}	4.1×10^{-14}	9.8×10^{-14}	4.9×10^{-12}	4.7×10^{-13}	7.6×10^{-14}
64	1.5×10^{-11}	1.8×10^{-12}	8.3×10^{-13}	2.0×10^{-11}	2.5×10^{-12}	5.3×10^{-13}
128	5.8×10^{-11}	5.3×10^{-13}	1.3×10^{-11}	5.4×10^{-10}	3.4×10^{-11}	1.9×10^{-13}
256	3.9×10^{-10}	1.2×10^{-10}	6.2×10^{-11}	1.2×10^{-08}	1.2×10^{-09}	1.7×10^{-11}
512	4.1×10^{-09}	6.5×10^{-10}	3.7×10^{-11}	1.5×10^{-07}	1.4×10^{-09}	1.9×10^{-11}

Table 7
The maximum absolute error for the second derivative of $f(x) = \sin x$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	7.8×10^{-12}	8.2×10^{-13}	6.5×10^{-13}	9.3×10^{-12}	1.0×10^{-12}	1.0×10^{-12}
32	2.1×10^{-10}	2.5×10^{-11}	1.5×10^{-11}	2.1×10^{-09}	2.8×10^{-10}	4.1×10^{-11}
64	1.2×10^{-08}	8.8×10^{-10}	1.1×10^{-09}	4.3×10^{-08}	2.1×10^{-09}	4.3×10^{-10}
128	2.6×10^{-07}	9.4×10^{-09}	9.4×10^{-09}	4.0×10^{-06}	2.4×10^{-08}	1.3×10^{-08}
256	7.4×10^{-06}	1.5×10^{-07}	1.5×10^{-07}	3.4×10^{-04}	2.8×10^{-06}	9.2×10^{-07}
512	3.4×10^{-04}	5.7×10^{-06}	5.7×10^{-06}	1.5×10^{-02}	2.4×10^{-04}	2.2×10^{-05}

Table 8
The maximum absolute error for the third derivative of $f(x) = \sin x$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	5.9×10^{-10}	3.4×10^{-11}	2.2×10^{-11}	3.6×10^{-10}	7.6×10^{-10}	2.0×10^{-10}
32	5.1×10^{-08}	3.2×10^{-09}	3.2×10^{-09}	4.6×10^{-07}	9.3×10^{-09}	3.2×10^{-09}
64	6.1×10^{-06}	3.1×10^{-07}	3.1×10^{-07}	4.3×10^{-05}	2.7×10^{-06}	1.7×10^{-07}
128	7.3×10^{-04}	1.7×10^{-05}	1.6×10^{-05}	1.4×10^{-02}	7.8×10^{-04}	1.1×10^{-04}
256	1.7×10^{-02}	1.4×10^{-03}	1.2×10^{-03}	$5.0 \times 10^{+00}$	4.2×10^{-01}	2.3×10^{-03}
512	1.5×10^{-01}	1.8×10^{-01}	1.8×10^{-01}	$8.3 \times 10^{+02}$	9.3×10^{-01}	9.2×10^{-01}

Table 9
The maximum absolute error for the fourth derivative of $f(x) = \sin x$

N	Eq. (14)	Eq. (15)	Eq. (16)	Eq. (2)	Eq. (3)	Eq. (4)
16	1.5×10^{-08}	1.4×10^{-09}	1.4×10^{-09}	2.0×10^{-08}	5.3×10^{-09}	4.1×10^{-09}
32	5.1×10^{-06}	4.5×10^{-07}	4.2×10^{-07}	7.1×10^{-05}	8.9×10^{-06}	7.1×10^{-07}
64	2.4×10^{-03}	2.3×10^{-04}	2.3×10^{-04}	2.8×10^{-02}	7.9×10^{-05}	6.4×10^{-04}
128	$1.5 \times 10^{+00}$	9.1×10^{-02}	9.9×10^{-02}	$3.5 \times 10^{+01}$	2.2×10^{-02}	1.0×10^{-01}
256	$6.6 \times 10^{+02}$	$1.3 \times 10^{+01}$	$1.3 \times 10^{+01}$	$4.9 \times 10^{+04}$	$4.6 \times 10^{+01}$	$5.5 \times 10^{+01}$
512	$5.3 \times 10^{+04}$	$8.2 \times 10^{+03}$	$8.7 \times 10^{+03}$	$3.2 \times 10^{+07}$	$6.2 \times 10^{+05}$	$1.2 \times 10^{+04}$

Appendix A

A.1. Error bound for the second order derivatives

Evaluating the elements of the second order differentiation matrix from Eq. (18) resulting roundoff error as yield

$$\begin{aligned}
d_{l,j}^{2*} - d_{l,j}^2 &= \frac{2\theta_j}{N} \sum_{k=2}^{N} \sum_{\substack{n=0\\(n+k)\ \text{even}}}^{k-2} \theta_k \frac{k(k^2-n^2)}{c_n} (-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]} \\
&\quad \times \left((\delta_{kj-N[\frac{kj}{N}]} + \delta_{nl-N[\frac{nl}{N}]}) - \mathrm{O}\left(\frac{1}{N^2}\delta_{kj-N[\frac{kj}{N}]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{nl-N[\frac{nl}{N}]}\right)\right) \\
&\leqslant \frac{4\theta_j}{3N}\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right) \sum_{k=2}^{N} \theta_k \left(k^4 - k^2\right) \\
&\leqslant \frac{4\theta_j}{3}\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\left(\frac{N^4}{5} - \frac{1}{5}\right),
\end{aligned}$$

from Eqs. (16) and (18) the elements of the first and last rows of the matrix $D^{(2)}$ can be computed by

$$d_{0j}^2 = \frac{2\theta_j}{3N} \sum_{k=2}^{N-1} (-1)^{[\frac{kj}{N}]} \left(k^4 - k^2\right) x_{kj-N[\frac{kj}{N}]} + \frac{(-1)^j \theta_j}{3}\left(N^3 - N\right),$$

with error upper bound

$$\begin{aligned}
d_{0j}^{2*} - d_{0j}^2 &= \frac{2\theta_j}{3N} \sum_{k=2}^{N-1} (-1)^{[\frac{kj}{N}]} \left(k^4 - k^2\right) \delta_{kj-N[\frac{kj}{N}]} \\
&\leqslant \frac{2\theta_j \delta}{3N} \sum_{k=2}^{N-1} (-1)^{[\frac{kj}{N}]} \left(k^4 - k^2\right) \leqslant \frac{2\delta}{3}\left(\frac{N^4}{5} - \frac{N^3}{2} + \frac{N}{2} - \frac{1}{5}\right).
\end{aligned}$$

Also, the element d_{01}^2 is the major elements concerning its values, where

$$d_{01}^{2*} - d_{01}^2 = \frac{2}{3N} \sum_{k=2}^{N-1} \left(k^4 - k^2\right) \delta_k \leqslant \frac{2\delta}{3}\left(\frac{N^4}{5} - \frac{N^3}{2} + \frac{N}{2} - \frac{1}{5}\right).$$

A.2. Error bounds for the third order derivatives

Adopting Eq. (19), the error on the elements $d^3_{l,j}$ is given by

$$\begin{aligned}
d^{3*}_{l,j} - d^3_{l,j} &= \frac{\theta_j}{N}\sum_{k=3}^{N}\sum_{\substack{n=0\\(n+k)\ \text{odd}}}^{k-3}\frac{\theta_k k}{2c_n}\left(p^2-1\right)\left(q^2-1\right)(-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]}\\
&\quad\times\left((\delta_{kj-N[\frac{kj}{N}]}+\delta_{nl-N[\frac{nl}{N}]}) - \mathrm{O}\left(\frac{1}{N^2}\delta_{kj-N[\frac{kj}{N}]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{nl-N[\frac{nl}{N}]}\right)\right)\\
&\leqslant \frac{\theta_j}{N}\left(\delta-\mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\sum_{k=3}^{N}\sum_{\substack{n=0\\(n+k)\ \text{odd}}}^{k-3}\frac{\theta_k k}{2c_n}\left(p^2-1\right)\left(q^2-1\right)\\
&\leqslant \theta_j\left(\delta-\mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\left(\frac{2N^6}{105}-\frac{N^4}{15}-\frac{N^2}{15}+\frac{4}{35}\right).
\end{aligned}$$

In view of Eqs. (16), (19) the elements of the first and last rows of the matrix $D^{(3)}$ are computed by

$$d^3_{0,j} = \frac{\theta_j}{N}\sum_{k=3}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^6}{15}-\frac{2k^4}{3}+\frac{8k^2}{15}\right)x_{kj-N[\frac{kj}{N}]} + \frac{(-1)^j\theta_j}{2}\left(\frac{2N^5}{15}-\frac{2N^3}{3}+\frac{8N}{15}\right).$$

This yields

$$\begin{aligned}
d^{3*}_{0j} - d^3_{0j} &= \frac{\theta_j}{N}\sum_{k=3}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^6}{15}-\frac{2k^4}{3}+\frac{8k^2}{15}\right)\delta_{kj-N[\frac{kj}{N}]}\\
&\leqslant \frac{\theta_j\delta}{N}\sum_{k=3}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^6}{15}-\frac{2k^4}{3}+\frac{8k^2}{15}\right)\\
&\leqslant \delta\left(\frac{2N^6}{105}-\frac{N^5}{15}-\frac{N^4}{15}+\frac{N^3}{3}-\frac{N^2}{15}-\frac{4N}{15}+\frac{4}{35}\right).
\end{aligned}$$

Also, the element d^3_{01} is the major elements concerning its values, where

$$d^{3*}_{01} - d^3_{01} = \frac{1}{N}\sum_{k=3}^{N-1}\left(\frac{2k^6}{15}-\frac{2k^4}{3}+\frac{8k^2}{15}\right)\delta_k \leqslant \delta\left(\frac{2N^6}{105}-\frac{N^5}{15}-\frac{N^4}{15}+\frac{N^3}{3}-\frac{N^2}{15}-\frac{4N}{15}+\frac{4}{35}\right).$$

A.3. Error bound for the fourth order derivatives

Considering Eq. (20), the error on the elements $d^4_{l,j}$ is given by

$$\begin{aligned}
d^{4*}_{l,j} - d^4_{l,j} &= \frac{\theta_j}{N}\sum_{k=4}^{N}\sum_{\substack{n=0\\(n+k)\ \text{even}}}^{k-4}\frac{\theta_k kpq}{12c_n}\left(p^2-4\right)\left(q^2-4\right)(-1)^{[\frac{kj}{N}]+[\frac{nl}{N}]}\\
&\quad\times\left((\delta_{kj-N[\frac{kj}{N}]}+\delta_{nl-N[\frac{nl}{N}]}) - \mathrm{O}\left(\frac{1}{N^2}\delta_{kj-N[\frac{kj}{N}]}\right) - \mathrm{O}\left(\frac{1}{N^2}\delta_{nl-N[\frac{nl}{N}]}\right)\right)
\end{aligned}$$

$$\leqslant \frac{\theta_j}{N}\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\sum_{k=4}^{N}\sum_{\substack{n=0\\(n+k)\ \text{even}}}^{k-4}\frac{\theta_k kpq}{12c_n}\left(p^2-4\right)\left(q^2-4\right)$$

$$\leqslant \theta_j\left(\delta - \mathrm{O}\left(\frac{1}{N^2}\delta\right)\right)\left(\frac{2N^8}{945} - \frac{8N^6}{315} + \frac{2N^4}{45} + \frac{124N^2}{945} - \frac{16}{105}\right).$$

In view of Eqs. (16) and (20), the elements of the first and last rows of the matrix $D^{(4)}$ are computed by

$$d_{0,j}^4 = \frac{\theta_j}{N}\sum_{k=4}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^8}{105} - \frac{4k^6}{15} + \frac{14k^4}{15} - \frac{24k^2}{35}\right)x_{kj-N[\frac{kj}{N}]} + \frac{(-1)^j\theta_j}{2}\left(\frac{2k^7}{105} - \frac{4k^5}{15} + \frac{14k^3}{15} - \frac{24k}{35}\right),$$

with error upper bound

$$d_{0j}^{4*} - d_{0j}^4 = \frac{\theta_j}{N}\sum_{k=4}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^8}{105} - \frac{4k^6}{15} + \frac{14k^4}{15} - \frac{24k^2}{35}\right)\delta_{kj-N[\frac{kj}{N}]}$$

$$\leqslant \frac{\theta_j\delta}{N}\sum_{k=4}^{N-1}(-1)^{[\frac{kj}{N}]}\left(\frac{2k^8}{105} - \frac{4k^6}{15} + \frac{14k^4}{15} - \frac{24k^2}{35}\right)$$

$$\leqslant \delta\left(\frac{2N^8}{945} - \frac{N^7}{105} - \frac{8N^6}{315} + \frac{2N^5}{15} + \frac{2N^4}{45} - \frac{7N^3}{15} + \frac{124N^2}{945} + \frac{12N}{35} - \frac{16}{105}\right).$$

Also, the element d_{01}^4 is the major elements concerning its values, where

$$d_{01}^{4*} - d_{01}^4 = \frac{1}{N}\sum_{k=4}^{N-1}\left(\frac{2k^8}{105} - \frac{4k^6}{15} + \frac{14k^4}{15} - \frac{24k^2}{35}\right)\delta_k$$

$$\leqslant \delta\left(\frac{2N^8}{945} - \frac{N^7}{105} - \frac{8N^6}{315} + \frac{2N^5}{15} + \frac{2N^4}{45} - \frac{7N^3}{15} + \frac{124N^2}{945} + \frac{12N}{35} - \frac{16}{105}\right).$$

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