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Letter to the editor

Numerical differentiation for high orders by an integration method☆

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ABSTRACT

This paper mainly studies the numerical differentiation by integration method proposed first by Lanczos. New schemes of the Lanczos derivatives are put forward for reconstructing numerical derivatives for high orders from noise data. The convergence rate of these proposed methods is $O\left(\delta^{\frac{4}{n+4}}\right)$ as the noise level $\delta \to 0$. Numerical examples show that the proposed methods are stable and efficient.

1. Introduction

Numerical differentiation provides a way of numerically determining the derivatives of an unknown function from its approximate values; and it is an important method in scientific research and engineering disciplines. For example, solutions related to image processing [1], magnetic resonance electrical impedance tomography [2,3] and identification [4] can be improved if the derivatives are obtained by a high accuracy approximation method. The problem of numerical differentiation is well known to be ill-posed, which means that the small errors in measurement data of the function can induce large errors in its computed derivatives. Therefore, various numerical methods have been suggested for obtaining the numerical derivatives [1,5–11]. These works mainly fall into four types: the mollification methods [5], the finite difference methods [6], the regularization methods [1,7,8] and the differentiation by integration methods [9–11]. The differentiation by integration methods, i.e. using the Lanczos generalized derivatives, are simple and effective methods firstly proposed by Lanczos [9].

The Lanczos generalized derivative [9] D_h, defined by

$$D_h f(x) = \frac{3}{2h^3}\int_{-h}^{h} t f(x+t)\mathrm{d}t = \frac{3}{2h}\int_{-1}^{1} t f(x+ht)\mathrm{d}t, \tag{1.1}$$

approximates $f'(x)$ in the sense $f'(x) = D_h f(x) + O(h^2)$. Recently, Rangarajana et al. [11] generalized it to the case for high order derivatives with

$$D_h^{(n)} f(x) = \frac{1}{h^n}\int_{-1}^{1} \rho_n(t) f(x+ht)\mathrm{d}t, \quad n = 1, 2, \ldots, \tag{1.2}$$

which is an approximation of the nth-order derivative $f^{(n)}(x)$ and obtained by choosing $\rho_n(t)$ such that

$$D_h^{(n)} f(x) = f^{(n)}(x) + O(h^2). \tag{1.3}$$

In fact, it is shown in [11] that $\rho_n(t)$ is proportional to the Legendre polynomial $P_n(t)$ by Taylor expansion, namely $\rho_n(t) = \gamma_n P_n(t)$, where $P_n(t)$ is the nth-order Legendre polynomial and $\gamma_n = \frac{1\times3\times5\times\cdots\times(2n+1)}{2}$.

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In this paper, we continue to work on the differentiation by integration methods to propose new schemes for obtaining the Lanczos derivatives for high orders. This paper is organized as follows: New schemes for obtaining the Lanczos derivatives for high orders are proposed with the corresponding convergence rate in Section 2. Numerical examples are given in Section 3 for verifying the efficiency and stability of the proposed schemes.

2. New schemes for obtaining high order derivatives

Introducing the following operator denoted by $D_h^{(n)}f$:

$$D_h^{(n)}f(x) = \frac{1}{h^n}\int_{-1}^{1} P_n(t)[\alpha_n f(x+ht) + \beta_n f(x+\lambda_n ht)]\mathrm{d}t, \tag{2.1}$$

where $P_n(t)$ is the nth-order Legendre polynomial, we choose α_n, β_n, λ_n such that

$$D_h^{(n)}f(x) = f^{(n)}(x) + O(h^4). \tag{2.2}$$

Since $P_n(-t) = (-1)^n P_n(t)$, we conclude that $D_h^{(n)}f(x) = D_{-h}^{(n)}f(x)$. So, we always take h to be positive in the following.

To get the rate of convergence of (2.1), we assume that $f(x)$ is bounded and has a continuous $(n+4)$th derivative on some interval I containing the points x, $x \pm h$, $x \pm \lambda_n h$. Assume further that $f^\delta(x)$ is some bounded integrable approximation of $f(x)$ satisfying

$$\|f^\delta(x) - f(x)\|_\infty = \sup_{x\in I}|f^\delta(x) - f(x)| \le \delta, \tag{2.3}$$

where δ is the noise level. To determine the coefficients α_n, β_n, λ_n, we write the Taylor expansion for a given n as follows:

$$\begin{aligned} f(x+ht) &= f(x) + htf'(x) + \cdots + \frac{h^n t^n}{n!}f^{(n)}(x) + \frac{h^{n+1}t^{n+1}}{(n+1)!}f^{(n+1)}(x) \\ &\quad + \frac{h^{n+2}t^{n+2}}{(n+2)!}f^{(n+2)}(x) + \frac{h^{n+3}t^{n+3}}{(n+3)!}f^{(n+3)}(x) + \frac{h^{n+4}t^{n+4}}{(n+4)!}f^{(n+4)}(\xi). \end{aligned} \tag{2.4}$$

Substituting (2.4) into (2.1) and noting the orthogonal property of Legendre polynomials, we know that

$$\frac{\alpha_n}{k!}\int_{-1}^{1} t^k P_n(t) + \frac{\beta_n\lambda_n^k}{k!}\int_{-1}^{1} t^k P_n(t)\mathrm{d}t = 0, \quad \forall k < n. \tag{2.5}$$

Furthermore, noting that

$$\frac{\alpha_n}{(k)!}\int_{-1}^{1} t^k P_n(t) + \frac{\beta_n\lambda_n^k}{(k)!}\int_{-1}^{1} t^k P_n(t)\mathrm{d}t = 0, \quad k = n+1, n+3, \tag{2.6}$$

we require that α_n, β_n, λ_n satisfy

$$\frac{\alpha_n}{n!}\int_{-1}^{1} t^n P_n(t)\mathrm{d}t + \frac{\beta_n\lambda_n^n}{n!}\int_{-1}^{1} t^n P_n(t)\mathrm{d}t = 1, \tag{2.7}$$

$$\frac{\alpha_n}{(n+2)!}\int_{-1}^{1} t^{n+2} P_n(t)\mathrm{d}t + \frac{\beta_n\lambda_n^{n+2}}{(n+2)!}\int_{-1}^{1} t^{n+2} P_n(t)\mathrm{d}t = 0. \tag{2.8}$$

Let $p_n = \int_{-1}^{1} t^n P_n(t)\mathrm{d}t$. From (2.7) and (2.8), we obtain

$$\begin{cases} \alpha_n + \beta_n\lambda_n^n = \dfrac{n!}{p_n}; \\ \alpha_n + \beta_n\lambda_n^{n+2} = 0. \end{cases} \tag{2.9}$$

By solving the system (2.9), we get

$$\alpha_n = -\frac{n!\lambda_n^2}{p_n(1-\lambda_n^2)}, \qquad \beta_n = \frac{n!}{p_n(\lambda_n^n - \lambda_n^{n+2})}. \tag{2.10}$$

From (2.10), λ_n is a free parameter. That is to say, there are infinitely varied schemes of (2.1) for computing the nth-order derivative. Does there exist an optimal λ_n? We will answer this problem in the sequel from the viewpoint of computation. Since $\int_{-1}^{1} t^{n+3}P_n(t)\mathrm{d}t = 0$, we have the following theorem from (2.4)–(2.8).

Theorem 1. *Let $f(x) \in C^{n+4}(I)$, and say there exists a positive constant M such that $|f^{(n+4)}(x)| \le M$. Then*

$$\|D_h^{(n)} f(x) - f^{(n)}(x)\|_\infty \le C_1 h^4,$$

where $C_1 = \frac{(|\alpha_n|+|\beta_n||\lambda_n^{n+4}|)M}{(n+4)!} \int_{-1}^{1} |t^{n+4} P_n(t)| \mathrm{d}t$, α_n, β_n and λ_n satisfy the system (2.9).

Theorem 2. *Let $f(x) \in C^{n+4}(I)$, and say there exists a positive constant M such that $|f^{(n+4)}(x)| \le M$. Then*

$$\|D_h^{(n)} f^\delta(x) - f^{(n)}(x)\|_\infty \le C_1 h^4 + C_2 \frac{\delta}{h^n},$$

where C_1 be the same constant of Theorem 1, $C_2 = (|\alpha_n| + |\beta_n|) \int_{-1}^{1} |P_n(t)| \mathrm{d}t$. Moreover, if we choose $h = d\delta^{\frac{1}{n+4}}$, then

$$\|D_h^{(n)} f^\delta(x) - f^{(n)}(x)\|_\infty = O\left(\delta^{\frac{4}{n+4}}\right), \quad \delta \to 0,$$

where d is a constant, α_n, β_n and λ_n satisfy the system (2.9).

Proof. Since

$$\|D_h^{(n)} f^\delta(x) - D_h^{(n)} f(x)\|_\infty = \left\| D_h^{(n)} \left(f^\delta(x) - f(x)\right)\right\|_\infty \le \frac{\delta}{h^n}(|\alpha_n| + |\beta_n|) \int_{-1}^{1} |P_n(t)| \mathrm{d}t,$$

one gets

$$\|D_h^{(n)} f^\delta(x) - f^{(n)}(x)\|_\infty \le \|D_h^{(n)} f(x) - f^{(n)}(x)\|_\infty + \|D_h^{(n)} f^\delta(x) - D_h^{(n)} f(x)\|_\infty \le C_1 h^4 + C_2 \frac{\delta}{h^n},$$

where $C_2 = (|\alpha_n| + |\beta_n|) \int_{-1}^{1} |P_n(t)| \mathrm{d}t$.

Let $\psi(h) = C_1 h^4 + C_2 \frac{\delta}{h^n}$. By simple calculation, the minimizer of $\psi(h)$ is

$$h^* = \left(\frac{nC_2\delta}{4C_1}\right)^{\frac{1}{n+4}} \tag{2.11}$$

and the minimum value is

$$\psi(h^*) = \frac{n+4}{4} \left(\frac{4}{n}\right)^{\frac{n}{n+4}} C_1^{\frac{n}{n+4}} C_2^{\frac{4}{n+4}} \delta^{\frac{4}{n+4}}. \tag{2.12}$$

Then, the proof is completed. □

Remark 3. In the proposed schemes (2.1), the convergence rate is improved from $O(h^2)$ to $O(h^4)$ for the exact function $f(x)$. Naturally, the convergence rate is improved from $O(\delta^{\frac{2}{n+2}})$ to $O(\delta^{\frac{4}{n+4}})$ for the noisy function if we choose $h = d\delta^{\frac{1}{n+4}}$, where d is a constant.

From the expression of C_1, C_2 and (2.10), by direct computation we can rewrite the minimum value $\psi(h^*)$ for fixed n as

$$\psi(h^*) = C_3 \left(\left|\frac{\lambda_n^2}{1-\lambda_n^2}\right| + \left|\frac{\lambda_n^{n+2}}{1-\lambda_n^n}\right|\right)^{\frac{n}{n+4}} \left(\left|\frac{\lambda_n^2}{1-\lambda_n^2}\right| + \left|\frac{1}{\lambda_n^2-\lambda_n^{n+2}}\right|\right) \delta^{\frac{4}{n+4}}, \tag{2.13}$$

where C_3 is a constant which depends on n and M.

Let

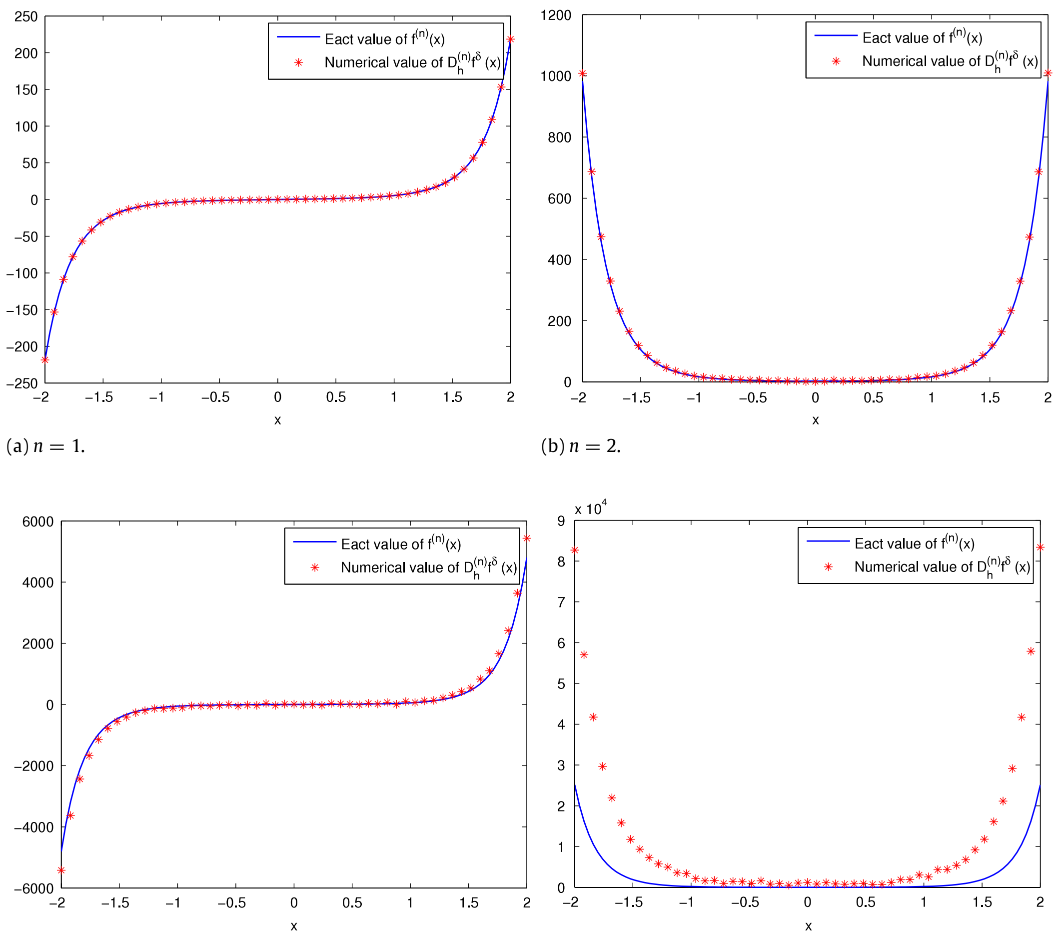
$$g(\lambda_n) \equiv \left(\left|\frac{\lambda_n^2}{1-\lambda_n^2}\right| + \left|\frac{\lambda_n^{n+2}}{1-\lambda_n^n}\right|\right)^{\frac{n}{n+4}} \left(\left|\frac{\lambda_n^2}{1-\lambda_n^2}\right| + \left|\frac{1}{\lambda_n^2-\lambda_n^{n+2}}\right|\right). \tag{2.14}$$

Therefore, we can choose an optimal λ_n^*, which is a minimizer of the function $g(\lambda_n)$, to minimize the minimum value $\psi(h^*)$ for fixed n. However, the minimizer of the function $g(\lambda_n)$ is not easy to obtain by methods of calculus. In view of the symmetry of $g(\lambda_n)$ and the practical applications, we only need to find the locally approximate minimizer by a discrete method. The locally optimal approximate minimizers of λ_n for different n, which are contained in the intervals $(0, 1)$ and $(1, 5)$ respectively, are shown in Table 1. It is interesting that the locally optimal values of λ_n decrease with n.

In the following, we investigate the convergence of the new scheme (2.1) for high order derivatives under assumptions on the function $f(x)$ that are weaker than $C^{n+4}(I)$. Obviously, it is easy to verify that the convergence rate is at least $O(h^k)+O(\frac{\delta}{h^n})$ if $f(x) \in C^{n+k}(I)$ and the derivative $f^{(n+k)}(x)$ of f is bounded for $k = 1, 2, 3$. In particular, $D_h^{(n)} f(x)$ converges to the

Table 1
Locally optimal approximation values of λ_n.

n	$\lambda_n^* \in (0, 1)$	$\lambda_n^* \in (1, 5)$	n	$\lambda_n^* \in (0, 1)$	$\lambda_n^* \in (1, 5)$
1	5.3242e−001	3.3917e+000	6	4.8771e−001	1.9567e+000
2	5.1067e−001	2.5488e+000	7	4.7892e−001	1.9166e+000
3	5.0352e−001	2.2541e+000	8	4.6860e−001	1.8879e+000
4	4.9938e−001	2.1044e+000	9	4.5744e−001	1.8667e+000
5	4.9449e−001	2.0150e+000	10	4.4611e−001	1.8507e+000



(a) $n = 1$.

(b) $n = 2$.

(c) $n = 3$.

(d) $n = 4$.

Fig. 1. The function $f_1^{(n)}(x)$ and its approximation $D_h^{(n)} f_1^{\delta}(x)$ for $\delta = 0.005$.

average value of the right and left hand derivatives for the nth order, supposing that $f(x) \in C^{n-1}(I)$ and these one-sided derivatives exist. In the following, we denote the right and left hand derivatives for the nth order as $f_+^{(n)}(x)$ and $f_-^{(n)}(x)$, respectively.

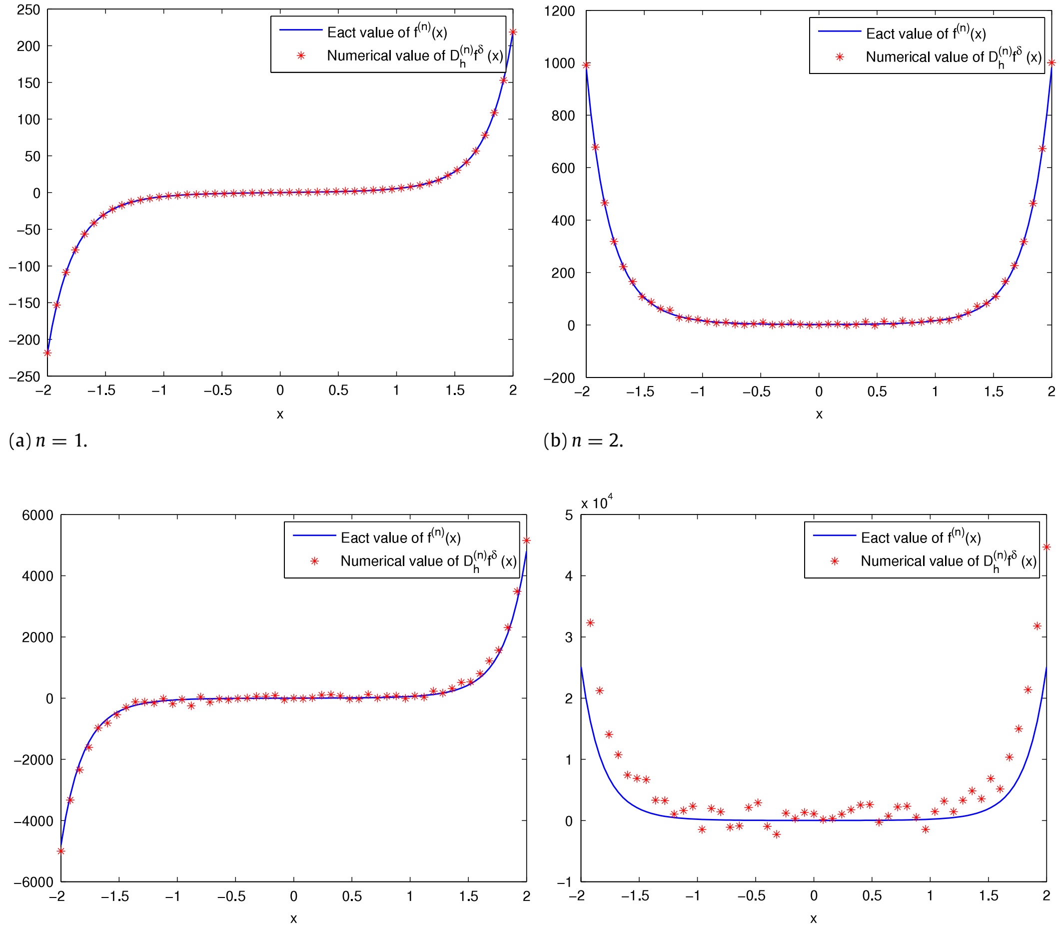
Theorem 4. *Let $f(x) \in C^{n-1}(I)$. If $f_+^{(n)}(x)$ and $f_-^{(n)}(x)$ exist at the point x, then*

$$\lim_{h \to 0} D_h^{(n)} f(x) = \frac{1}{2}\left(f_-^{(n)}(x) + f_+^{(n)}(x)\right), \tag{2.15}$$

where α_n, β_n and λ_n satisfy the system (2.9).

Proof. By the local Taylor formula with the Peano remainder term [12], for any given $\varepsilon > 0$, there exists $\delta > 0$ such that

$$\left| f(x+t) - Q(t) - \frac{f_-^{(n)}(x)}{n!} t^n \right| < \varepsilon |t|^n, \quad -\delta < t < 0 \tag{2.16}$$



(a) $n = 1$. (b) $n = 2$.

(c) $n = 3$. (d) $n = 4$.

Fig. 2. The function $f_1^{(n)}(x)$ and its approximation $D_h^{(n)} f_1^{\delta}(x)$ for $\delta = 0.05$.

and

$$\left| f(x+t) - Q(t) - \frac{f_+^{(n)}(x)}{n!} t^n \right| < \varepsilon t^n, \quad 0 < t < \delta, \tag{2.17}$$

where $Q(t) = f(x) + \frac{f'(x)}{1!} t + \frac{f''(x)}{2!} t^2 + \cdots + \frac{f^{(n-1)}(x)}{(n-1)!} t^{n-1}$.

Since $\alpha_n, \beta_n, \lambda_n$ satisfy the system (2.9) and $\int_0^1 t^n P_n(t) \mathrm{d}t = \int_{-1}^0 t^n P_n(t) \mathrm{d}t$, we have

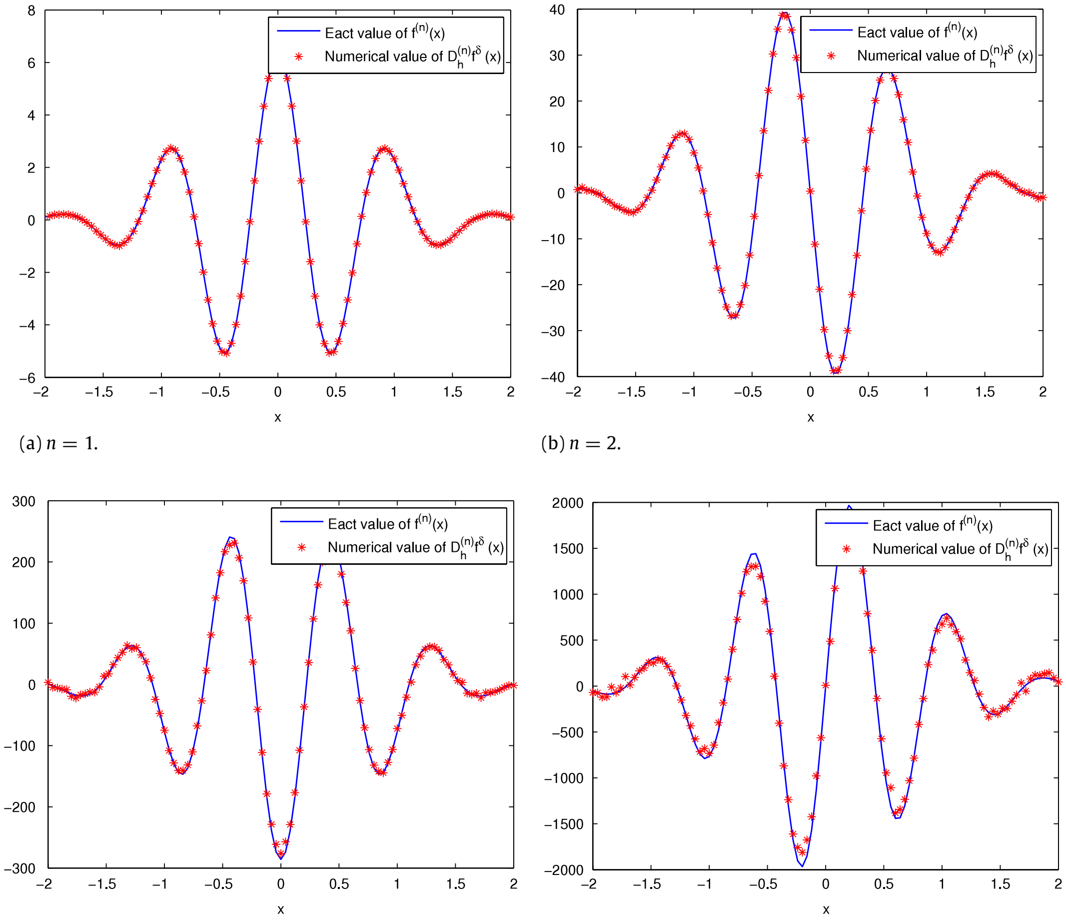
$$\frac{1}{h^n} \int_0^1 P_n(t) \left[\alpha_n \frac{f_+^{(n)}(x)}{n!} (ht)^n + \beta_n \frac{f_+^{(n)}(x)}{n!} (\lambda_n h t)^n \right] \mathrm{d}t = \frac{1}{2} f_+^{(n)}(x) \tag{2.18}$$

and

$$\frac{1}{h^n} \int_{-1}^0 P_n(t) \left[\alpha_n \frac{f_-^{(n)}(x)}{n!} (ht)^n + \beta_n \frac{f_-^{(n)}(x)}{n!} (\lambda_n h t)^n \right] \mathrm{d}t = \frac{1}{2} f_-^{(n)}(x). \tag{2.19}$$

On the other hand, according to the orthogonality of Legendre polynomials we obtain

$$\frac{1}{h^n} \int_{-1}^1 P_n(t) [\alpha_n Q(ht) + \beta_n Q(\lambda_n h t)] \mathrm{d}t = 0. \tag{2.20}$$



(a) $n = 1$. (b) $n = 2$.

(c) $n = 3$. (d) $n = 4$.

Fig. 3. The function $f_2^{(n)}(x)$ and its approximation $D_h^{(n)} f_2^{\delta}(x)$ for $\delta = 0.005$.

From (2.16)–(2.20) and noting that $|P_n(t)| \le 1$ for $t \in [-1, 1]$, we have by simple computation

$$\left| D_h^{(n)} f(x) - \frac{1}{2}[f_-^{(n)}(x) + f_+^{(n)}(x)] \right| \le \frac{2(|\alpha_n| + |\beta_n||\lambda_n|^n)}{n+1} \varepsilon$$

for $0 < \max\{h|t|, h|\lambda_n||t|\} < \delta$. Since $D_h^{(n)} f(x) = D_{-h}^{(n)} f(x)$, we conclude that

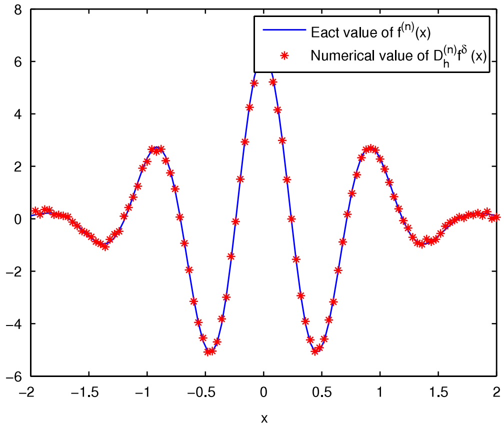
$$\lim_{h \to 0} D_h^{(n)} f(x) = \frac{1}{2}\left(f_-^{(n)}(x) + f_+^{(n)}(x) \right).$$

Then, the proof is completed. □

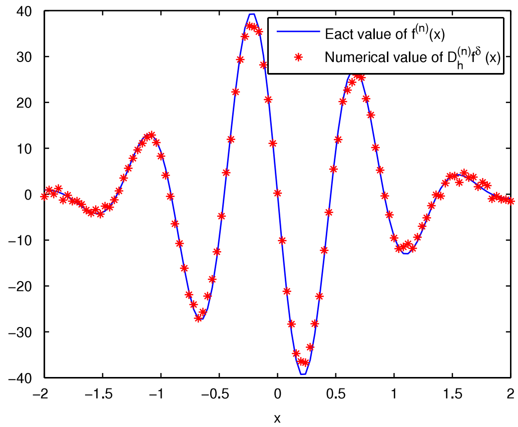
3. Numerical examples

In this section, we give three examples to verify the effect of the new schemes. They are two smooth functions and a non-smooth function. All codes are written in Matlab. Noise data are generated by $f^{\delta}(x) = f(x) + \delta \cdot R(x)$, where δ is the noise level, and $R(x)$ is a random function with zero mean value and standard deviation $\sigma = 1$ and generated by the built-in function "randn". The integral (2.1) is computed at 101 equally spaced values $t \in [-1, 1]$ by using the trapezoidal method. Figs. 1–5 are plotted by taking the approximately optimal values $\lambda_n^* \in (0, 1)$ from Table , and $h = h^* = (\frac{nC_2\delta}{4C_1})^{1/(n+4)}$ depending on λ_n^*. Thus, the derivatives at the point $x \in [a, b]$ are computed from the $f(x)$ data on the interval $[a - h, b + h]$. In the following examples, we always fix $a = -2$, $b = 2$.

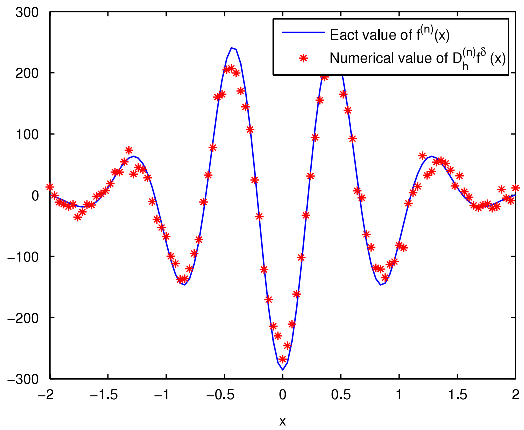
To compare performances for the choice $\lambda_n^* \in (0, 1)$ and the choice $\lambda_n^* \in (1, 5)$, we provide the errors $\|D_h^{(n)} f^{\delta}(x) - f^{(n)}(x)\|_{\infty}$ in Table 2 for the functions $f_1(x), f_2(x)$ that satisfy the condition $f(x) \in C^{n+4}(I)$. The values of Table 2 are obtained by using noise level $\delta = 0.005$ and the same noise data generated by the Matlab function "randn" with STATE reset to 0.



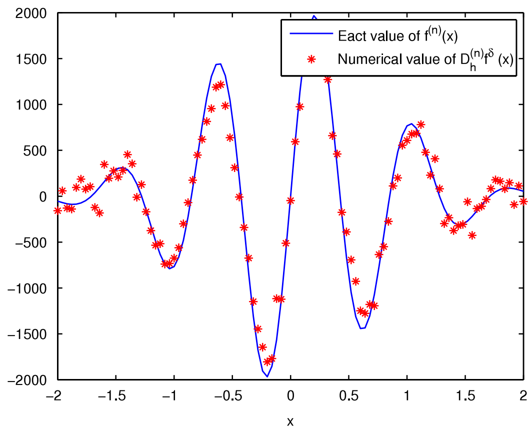
(a) $n = 1$.



(b) $n = 2$.



(c) $n = 3$.



(d) $n = 4$.

Fig. 4. The function $f_2^{(n)}(x)$ and its approximation $D_h^{(n)} f_2^{\delta}(x)$ for $\delta = 0.05$.

Table 2

Errors $\|D_h^{(n)} f^{\delta} - f^{(n)}\|_{\infty}$ for $\lambda_n^* \in (0, 1)$ and $\lambda_n^* \in (1, 5)$ with $\delta = 0.005$.

$f(x)$	n	1	2	3	4
$f_1(x)$	$\lambda_n^* \in (0, 1)$	4.6643e−002	2.4631e+001	6.2629e+002	5.6343e+004
$f_1(x)$	$\lambda_n^* \in (1, 5)$	4.7997e−002	2.6377e+001	6.3639e+002	5.7059e+004
$f_2(x)$	$\lambda_n^* \in (0, 1)$	2.1096e−002	5.2504e−001	1.0911e+001	1.8942e+002
$f_2(x)$	$\lambda_n^* \in (1, 5)$	2.6317e−002	6.1763e−001	1.1805e+001	1.9397e+002

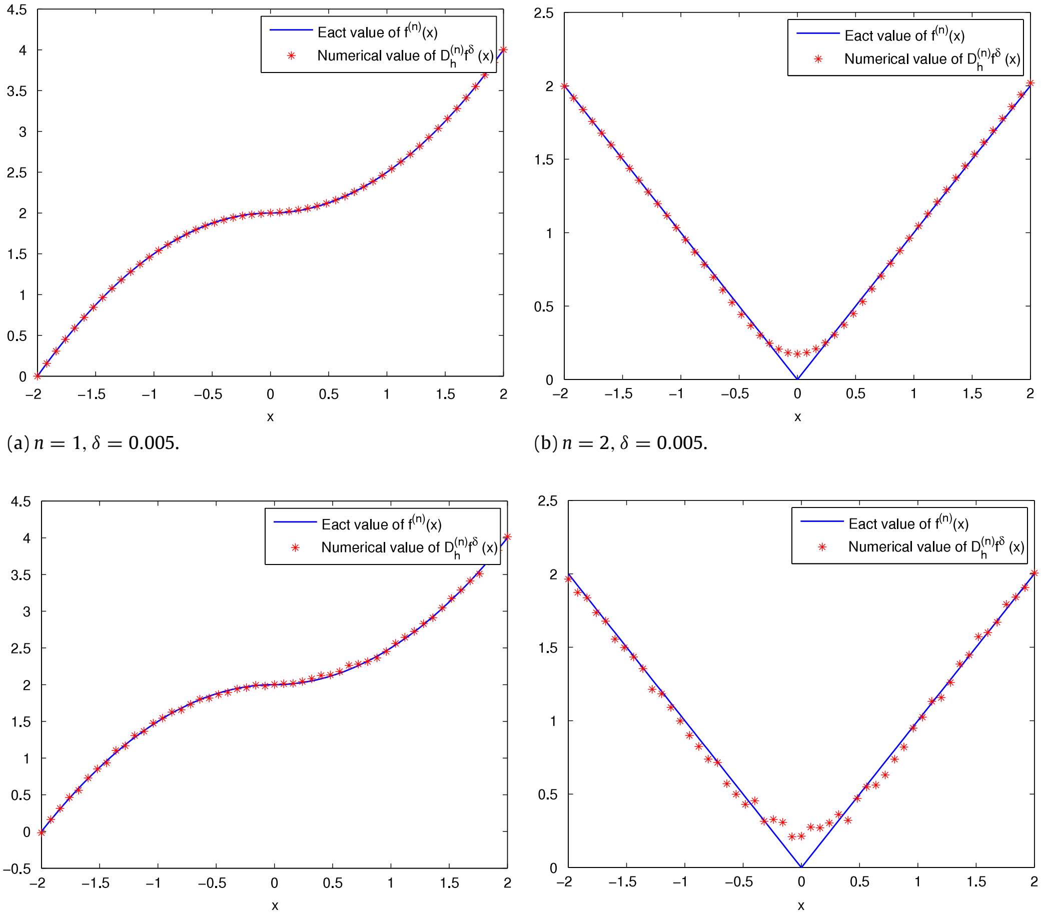
The results of Table 2 show that the choice $\lambda_n^* \in (0, 1)$ is better than the choice $\lambda_n^* \in (1, 5)$. For other random noise data, we also verify that the above conclusion is correct.

Example 1. The exact function is chosen as $f_1(x) = e^{x^2}$. The numerical results are shown in Figs. 1 and 2 in which the solid lines represent $f_1^{(n)}(x)$ and the star $(*)$ lines represent $D_h^{(n)} f_1^{\delta}(x)$. The noise level is $\delta = 0.005$ in Fig. 1 while it is $\delta = 0.05$ in Fig. 2.

Example 2. The exact function is chosen as $f_2(x) = \sin(2\pi x)e^{-x^2}$. The numerical results are shown in Figs. 3 and 4 in which the solid lines represent $f_2^{(n)}(x)$ and the star $(*)$ lines represent $D_h^{(n)} f_2^{\delta}(x)$. The noise level is $\delta = 0.005$ in Fig. 3 while it is $\delta = 0.05$ in Fig. 4.

Example 3. Consider a non-smooth function

$$f_3(x) = \begin{cases} -\dfrac{1}{6}x^3 + 2x, & x \le 0, \\ \dfrac{1}{6}x^3 + 2x, & x > 0. \end{cases}$$



(a) $n = 1$, $\delta = 0.005$.
(b) $n = 2$, $\delta = 0.005$.
(c) $n = 1$, $\delta = 0.05$.
(d) $n = 2$, $\delta = 0.05$.

Fig. 5. The function $f_3^{(n)}(x)$ and its approximation $D_h^{(n)} f_3^{\delta}(x)$.

Its second derivative is $f_3''(x) = |x|$, and its third derivative at the point $x = 0$ does not exist. So, this function does not satisfy the condition $f(x) \in C^{n+4}(I)$ of Theorem 2. The numerical results are shown in Fig. 5 in which the solid lines represent $f_3^{(n)}(x)$ and the star $(*)$ lines represent $D_h^{(n)} f_3^{\delta}(x)$. Fig. 5(a)–(b) are computed with the noise level $\delta = 0.005$, and Fig. 5(c)–(d) are plotted for $\delta = 0.05$.

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