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Legendre Polynomials-Based Numerical Differentiation: A Convergence Analysis in a Weighted L^2 Space

Qin FANG[1], **Haojie LI**[1], **Min XU**[2,*]

1. *College of Information and Engineering, Dalian University, Liaoning* 116600*, P. R. China;*
2. *School of Mathematical Sciences, Dalian University of Technology, Liaoning* 116024*, P. R. China*

Abstract We consider the problem of estimating the derivative of a function f from its noisy version f^δ by using the derivatives of the partial sums of Fourier-Legendre series of f^δ. Instead of the observation L^2 space, we perform the reconstruction of the derivative in a weighted L^2 space. This takes full advantage of the properties of Legendre polynomials and results in a slight improvement on the convergence order. Finally, we provide several numerical examples to demonstrate the efficiency of the proposed method.

Keywords Legendre polynomials; numerical differentiation; Jacobi polynomials; weighted L^2 space

MR(2010) Subject Classification 65D25

1. Introduction

Numerical differentiation is a problem consisting in estimating the derivative f' of a function f from the noisy measurement f^δ which is not assumed to be differentiable. It arises from many scientific researches and applications, and is discussed extensively in computational mathematics [1–3]. At the same time, such a problem is known to be ill-posed in the sense that small errors in the measurement of a function may lead to large errors in its computed derivatives [4]. A number of special techniques have been developed for numerical differentiation.

For example, if f^δ admits the evaluation at any point $x \in [-1,1]$, then one may think of it as $f^\delta \in C[-1,1]$ and apply a variety of properly regularized numerical differentiation techniques (see e.g., [5,6] and references therein). However, f^δ can sometimes only be given by a finite set of noisy Fourier coefficients

$$f_k^\delta = \langle f^\delta, \varphi_k \rangle_{L^2} := \int_{-1}^{1} f^\delta(x)\varphi_k(x)\mathrm{d}x, \quad k = 0, 1, \ldots, N, \tag{1}$$

with respect to some orthonormal system $\{\varphi_k(x)\}_{k=0}^\infty$, which is called a design. In such a case, a general assumption is that $f^\delta \in L^2(-1,1)$ and

$$\|f - f^\delta\|_{L^2} \le \delta, \tag{2}$$

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* Corresponding author
E-mail address: wolf_hsu@dlut.edu.cn (Min XU)

where δ is used for measuring the noise level. One is sometimes advised to find f', by means of the standard regularization methods, from the ill-posed integral equation

$$A(f')(x) := \int_{-1}^{x} f'(u)\mathrm{d}u = f^{\delta}(x) - f^{\delta}(-1). \tag{3}$$

However, according to Example 5 of [7], even if one uses the native design $\{\varphi_k(x)\}_{k=0}^{\infty}$ of the operator A consisting of its singular functions, the derivatives of some simple and analytic functions cannot be reconstructed by using the standard regularization methods with L^2 accuracy better than $\mathcal{O}(\delta^{\frac{1}{3}})$. Thus, it is not always reasonable to transform the problem of numerical differentiation into the equation (3).

Recently, an alternative numerical differentiation method by using Legendre polynomials was developed in [8]. Let $L_k(x)$ denote k-th Legendre polynomials:

$$L_k(x) = (-1)^k \sqrt{k+1/2}(2^k k!)^{-1} \frac{\mathrm{d}^k}{\mathrm{d}x^k}\{(1-x^2)^k\}, \quad k = 0, 1, \ldots.$$

It is well known that the polynomials $\{L_k(x)\}_{k=0}^{\infty}$ are L^2-orthonormal on $[-1, 1]$, i.e.,

$$\int_{-1}^{1} L_k(x)L_m(x)\mathrm{d}x = \delta_{k,m},$$

where $\delta_{k,m}$ is the Kronecker delta. With the assumptions (1) and (2), the authors consider the approximation of $f'(x)$ by using the derivatives of the partial sums of Fourier-Legendre series of f^{δ}

$$S_n f^{\delta}(x) := \sum_{k=0}^{n} f_k^{\delta} L_k(x),$$

where $f_k^{\delta} = \langle f^{\delta}, L_k\rangle_{L^2}$. Consequently, the numerical differentiation scheme takes the form

$$D_n f^{\delta}(x) := \frac{\mathrm{d}}{\mathrm{d}x}(S_n f^{\delta}(x)) = \sum_{k=1}^{n} f_k^{\delta} L_k'(x). \tag{4}$$

The error estimates for the scheme (4) are considered in the observation space $L^2(-1, 1)$ as well as the space of continuous functions $C[-1, 1]$.

We note here that the derivatives of Legendre polynomials $L_k'(x)$ in (4) are proportional to the Jacobi polynomials $P_{k-1}^{(1,1)}(x)$ given by

$$P_{k-1}^{(1,1)}(x) = \sqrt{(k+1)(k+3/2)(k+2)} \frac{(-1)^k}{2^{k+1}(k+1)!} \frac{1}{(1-x^2)} \frac{\mathrm{d}^k}{\mathrm{d}x^k}\{(1-x^2)^{k+1}\}.$$

To be more precise, we have

$$L_k'(x) = \sqrt{k(k+1)} P_{k-1}^{(1,1)}(x), \quad k \geq 1. \tag{5}$$

On the other hand, the sequence $\{P_k^{(1,1)}(x)\}_{k=0}^{\infty}$ is orthonormal with respect to the weight function $w(x) = 1 - x^2$ (see [9] for details):

$$\int_{-1}^{1} P_k^{(1,1)}(x) P_m^{(1,1)}(x) w(x)\mathrm{d}x = \delta_{k,m}, \quad k, m \geq 0. \tag{6}$$

Thus, compared with the space L^2, it would be more beneficial to consider the numerical differentiation scheme (4) in the weighted space L_w^2. As we shall see later, this will take full advantage of the properties of the derivatives of Legendre polynomials, and lead to a slight improvement on the convergence order.

The rest of this paper is structured as follows. Section 2 contains the main results for the reconstruction of derivative of functions in the weighted L^2_w space and the corresponding error estimates. Using an adaptive rule based on the balancing principle for choosing the regularization parameter n, we present in Section 3 the numerical experiments supporting our main results.

2. Main results

To estimate the accuracy of the numerical differentiation (4) in the L^2_w sense, we need a quantitative measure of smoothness of the function f to be differentiated. As done in the paper [8], we measure the smoothness of the function f by decay of its Fourier-Legendre coefficients $f_k = \langle f, L_k\rangle_{L^2}$. Let $\psi : [0,\infty) \to [0,\infty)$ be a non-decreasing continuous function satisfying $\lim_{x\to\infty} \psi(x) = \infty$. We assume that f belongs to the space

$$W_2^{\psi} := \Big\{ g : g \in L^2(-1,1), \|g\|_{\psi}^2 = \sum_{k=0}^{\infty} \psi^2(k) |\langle g, L_k\rangle_{L^2}|^2 < \infty \Big\}. \tag{7}$$

This assumption allows us to treat simultaneously the cases of finite and infinite smoothness, which correspond to ψ increasing with polynomial and exponential rate, respectively. For example, let W_2^{μ} denote the space W_2^{ψ} with $\psi(x) = x^{\mu}$, and let H_2^r be the Sobolev space of L^2 functions whose weak derivatives of order up to r are also in $L^2(-1,1)$. It was shown in [10] that for $r \ge \mu$, $H_2^r \subset W_2^{\mu}$.

From the above discussion, one can easily see that the error between $f'(x)$ and its approximation $D_n f^{\delta}(x)$ can be bounded in L^2_w norm as follows

$$\|f' - D_n f_{\delta}\|_{L^2_w} \le \|f' - D_n f\|_{L^2_w} + \|D_n f - D_n f^{\delta}\|_{L^2_w}. \tag{8}$$

The first term in the right-hand side of (8) is called the approximation error, and the second term is called the noise propagation error. We shall estimate these terms for $f \in W_2^{\psi}$ and specify our estimates for ψ increasing with polynomial or exponential rate.

Let us first estimate the approximation error.

Lemma 2.1 *Let $f \in W_2^{\psi}$. Then the approximation error has the following bound*

$$\|f' - D_n f\|_{L^2_w} \le \Big(\sup_{k \ge n+1} \frac{k(k+1)}{\psi^2(k)} \Big)^{\frac{1}{2}} \|f\|_{\psi}. \tag{9}$$

In case $\psi(x) = x^{\mu}$ ($\mu > 2$) and $\psi(x) = e^{xh}$ ($h > 0$), the bound (9) reduces to the following ones respectively:

$$\|f' - D_n f\|_{L^2_w} \le \sqrt{\frac{n+2}{n+1}} (n+1)^{1-\mu} \|f\|_{\psi}, \tag{10}$$

and

$$\|f' - D_n f\|_{L^2_w} \le \sqrt{(n+1)(n+2)}\, e^{-(n+1)h} \|f\|_{\psi}. \tag{11}$$

Proof From (4) and (5), we have

$$f'(x) - (D_n f)(x) = f'(x) - \sum_{k=1}^{n} \langle f, L_k\rangle_{L^2} L_k'(x) = \sum_{k=n+1}^{\infty} \langle f, L_k\rangle_{L^2} L_k'(x)$$

$$= \sum_{k=n+1}^{\infty} \langle f, L_k\rangle_{L^2} \sqrt{k(k+1)} P_{k-1}^{(1,1)}(x).$$

It follows from (6) and (7) that

$$\begin{aligned}\|f' - D_n f\|_{L_w^2}^2 &= \int_{-1}^{1} \Big(\sum_{k=n+1}^{\infty} \langle f, L_k\rangle_{L^2} \sqrt{k(k+1)} P_{k-1}^{(1,1)} \Big)^2 w(x)\mathrm{d}x \\ &= \sum_{k=n+1}^{\infty} |\langle f, L_k\rangle_{L^2}|^2 k(k+1) \\ &= \sum_{k=n+1}^{\infty} |\langle f, L_k\rangle_{L^2}|^2 \psi^2(k) \frac{k(k+1)}{\psi^2(k)} \\ &\le \Big(\sup_{k\ge n+1} \frac{k(k+1)}{\psi^2(k)} \Big) \|f\|_{\psi},\end{aligned}$$

which proves the bound (9). A routine calculation gives rise to (10) and (11).

Next we estimate the noise propagation error.

Lemma 2.2 *Under the assumption (2), the following bound holds true*

$$\|D_n f - D_n f^{\delta}\|_{L_w^2} \le \sqrt{n(n+1)}\delta. \tag{12}$$

Proof Let $c_k = \langle f - f^{\delta}, L_k\rangle_{L^2}$ $(k \ge 0)$. In view of (2), it follows that

$$\sum_{k=0}^{\infty} c_k^2 = \|f - f^{\delta}\|_{L^2} \le \delta^2.$$

From (5), we have

$$D_n f - D_n f^{\delta} = \sum_{k=1}^{n} c_k L_k'(x) = \sum_{k=1}^{n} c_k \sqrt{k(k+1)} P_{k-1}^{(1,1)}(x).$$

Then

$$\begin{aligned}\|D_n f - D_n f^{\delta}\|_{L_w^2}^2 &= \int_{-1}^{1} \Big(\sum_{k=1}^{n} c_k \sqrt{k(k+1)} P_{k-1}^{(1,1)}(x) \Big)^2 w(x)\mathrm{d}x \\ &= \sum_{k=1}^{n} c_k^2 k(k+1) \le n(n+1) \sum_{k=1}^{n} c_k^2 \le n(n+1)\delta^2.\end{aligned}$$

Extracting the square root, we get (12). □

Using Lemmas 2.1 and 2.2, we obtain our main result immediately. In what follows C stands for some absolute positive constant, which may not be the same at different occurrences.

Theorem 2.3 *Let the assumption (2) be satisfied. If $f \in W_2^{\psi}$ with $\psi(x) = x^{\mu}$, then for $\mu > 2$ there exists a number n of the form $n = \lfloor C\delta^{\frac{1}{1-\mu}} \rfloor - 1$ such that*

$$\|f' - D_n f^{\delta}\|_{L_w^2} = \mathcal{O}(\delta^{\frac{\mu-2}{\mu-1}}). \tag{13}$$

Suppose that $f \in W_2^{\psi}$ with $\psi(x) = e^{xh}$ $(h > 0)$. Then there exists a number n of the form $n = \lfloor C\frac{1}{h}\log\frac{1}{\delta} \rfloor$ such that

$$\|f' - D_n f^{\delta}\|_{L_w^2} = \mathcal{O}(\delta \log \frac{1}{\delta}). \tag{14}$$

Remark 2.4 Under the same condition as in Theorem 2.3, it was shown in [8] that for $f \in W_2^{\psi}$ with $\psi(x) = x^{\mu}$ ($\mu > 2$), then one has

$$\|f' - D_n f^{\delta}\|_{L^2} = \mathcal{O}(\delta^{\frac{\mu-2}{\mu}});$$

in addition, for $f \in W_2^{\psi}$ with $\psi(x) = e^{xh}$ ($h > 0$), one has

$$\|f' - D_n f^{\delta}\|_{L^2} = \mathcal{O}(\delta \log^2 \delta).$$

Therefore, the estimations (13) and (14) imply that the reconstruction of the derivative in the weighted space L_w^2 could lead to a slight improvement on the convergence order.

Remark 2.5 Note that n plays the role of the regularization parameter in the method $D_n f^{\delta}$. With the noise propagation error bound (12) at hand, we can choose n based on the so-called balancing principle as follows

$$n_+ = \min\big\{n : \|D_n f^{\delta} - D_m f^{\delta}\|_{L_w^2} \le 4\sqrt{m(m+1)}\delta, m = N, N-1, \ldots, n+1\big\}. \qquad (15)$$

Using the deterministic oracle inequality [10], one can show easily that the choice $n = n_+$ gives an error bound that only by a constant factor worse than the best possible one.

3. Numerical experiments

In this section, we use two numerical experiments to demonstrate the method $D_n f^{\delta}$ together with the adaptive parameter choice rule (15). In particular, we shall compare our method with that performed in the space $L^2(-1, 1)$, namely, the method $D_n f^{\delta}$ together with the parameter choice rule:

$$n_+ = \min\big\{n : \|D_n f^{\delta} - D_m f^{\delta}\|_{L_w^2} \le 4\lambda(m)\delta, m = N, N-1, \ldots, n+1\big\}, \qquad (16)$$

where $\lambda(m) = \frac{1}{2} m\sqrt{m^2 + 6m + 5}$.

Set the largest truncation level $N = 50$. Noisy coefficients $\{f_i^{\delta}\}_{i=1}^n$ are simulated as follows. First, calculate the values of a function f at 400 points x_i which are uniformly distributed in $[-1, 1]$. Then, using the least squares method, find the coefficients of the linear combination $\sum_{i=0}^n c_i L_i(x)$ from the data $(x_i, f(x_i))$, $i = 1, 2, \ldots, 400$. Finally, take $f_i^{\delta} = c_i + \xi_i^{\delta}$, $i = 0, 1, \ldots, 50$, where ξ_i^{δ} is distributed according to the normal distribution.

We consider the following functions on $[-1, 1]$:

$$f_1(x) = \big(1 - \frac{2}{3}x + \frac{1}{9}\big)^{-\frac{1}{2}}, \quad f_1'(x) = \frac{1}{3}\big(1 - \frac{2}{3}x + \frac{1}{9}\big)^{-\frac{3}{2}};$$
$$f_2(x) = x^2, \quad f_2'(x) = 2x.$$

The numerical results of the derivative approximation with different truncation levels n_+ for $\delta = 10^{-3}$ and $\delta = 10^{-2}$ are shown in Figures 1 and 2, respectively. The approximated derivatives with the truncation levels chosen in accordance with (15) and (16) are depicted respectively in the right panels and left ones. It can be seen from Figures 1 and 2 that, the truncated derivative method $D_n f^{\delta}$ with the parameter choice rule (15) could outperform the method $D_n f^{\delta}$ with the parameter choice rule (16).

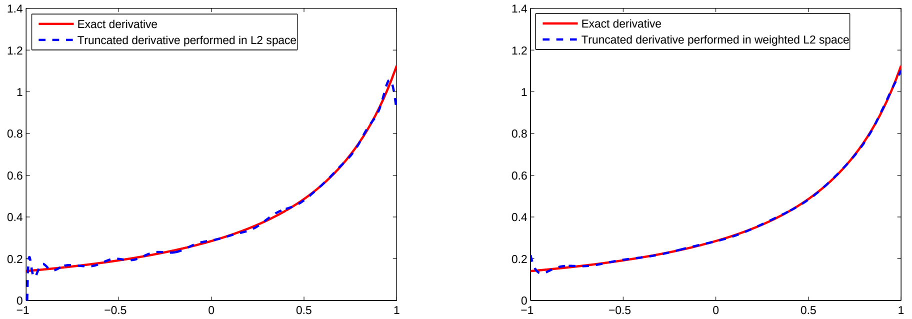

Figure 1 Numerical results on $[-1,1]$ for f_1. Left: the approximated derivative performed in the L^2 space with the truncation level $n_+ = 29$. Right: the approximated derivative performed in the weighted L^2 space with the truncation level $n_+ = 17$.

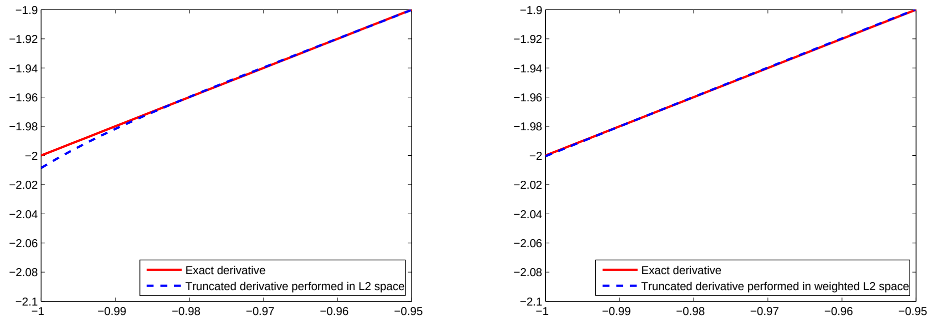

Figure 2 Numerical results near $x = -1$ for f_2. Left: the approximated derivative performed in the L^2 space with the truncation level $n_+ = 29$. Right: the approximated derivative performed in the weighted L^2 space with the truncation level $n_+ = 17$.

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