Numerical Differentiation of 2D Functions by a Mollification Method Based on Legendre Expansion

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Abstract

In this paper, we consider numerical differentiation of bivariate functions when a set of noisy data is given. A mollification method based on spanned by Legendre polynomials is proposed and the mollification parameter is chosen by a discrepancy principle. The theoretical analyses show that the smoother the genuine solution, the higher the convergence rates of the numerical solution. To get a practical approach, we also derive corresponding results for Legendre-Gauss-Lobatto interpolation. Numerical examples are also given to show the efficiency of the method.

Keywords: *Ill-posed problem, Numerical differentiation, Legendre spectral method, Discrepancy principle.*

1. Introduction

Numerical differentiation is a problem of determining the derivatives of a function from its perturbed values on an interval or some scattered points. It arises from many scientific research projects and applications, e.g., the identification of the discontinuous points in an image process [1]; the problem of solving the Abel integral equation [2, 3]; the problem of determining the peaks in chemical spectroscopy [4] and some inverse problems in mathematical physics [5], etc. The main difficulty is that differentiation is an ill-posed problem, which means small errors in the measurement of a function may lead to large errors in its computed derivatives [5, 6]. Some computational methods have been suggested for one-dimensional case [5-9, 11, 12], but so far only a very few results on the high dimensional case have been reported [13-16] and most of these papers focus on the first order derivative. As far as we know, the literature on higher order differentiation in two dimensions is extremely poor. In [14], G. Nakamura, S. Z. Wang and Y. B. Wang proposed a method for constructing second order derivatives of 2D functions. They have present a convergence result for functions in $H^4(\Omega)$ and the convergence rate can not be improved even if the functions have a higher smoothness. Moreover, an additional boundary condition is needed for their method.

In the present paper, as an alternative way of dealing with numerical differentiation, we introduce a new mollification method. Mollification methods for the regularization of ill-posed problems have been studied and analysed in a number of publications, whereof we can only cite a short list [8, 9, 17-20]. Generally, the idea of mollification methods for an evaluation problem.

$$y = Ax$$

with perturbed data x^δ , $\|x^\delta - x\| \le \delta$ (δ is is a known error level) consists of two stages:

- Take the mollification of x^δ :
$$x^\delta \to M_\alpha x^\delta .$$
- Take
$$y_\alpha^\delta = AM_\alpha x^\delta$$
as the approximation of y .

The key issues of mollification methods are construction of the mollification operator M_α and choice of the mollification parameter α . In this paper, we will construct the mollification operator by using subspace projection associated with Legendre polynomials. We also point out that the mollification parameter can be chosen by a general strategy----the discrepancy principle, which has been thoroughly studied [6,21,22]. The theoretical analysis shows that the smoother the genuine solution, the higher the convergence rate of the numerical solution. Moreover, the solution processes will be uniform in our method for the different order derivatives and the method is self-adaptive.

This paper is organized as follows. In section 2, we present some preliminary materials which will be used throughout the paper. The methods to construct approximate functions by Legendre expansion and Legendre-Gauss-Lobatto interpolation will be found in section 3 and 4. Some numerical results are given in section 5 to show the efficiency of the new methods.

2. Preliminaries

In this section, we present some preliminary materials which will be used throughout the paper. Let (x_1, x_2) and $\Omega = (-1,1)\times(-1,1)$ and denote by $L^2(\Omega)$ and $H^r(\Omega)$ the usual Lebesgue and Sobolev spaces and by $\|v\|$, $\|v\|_r$ their corresponding norm. Let N be the set of all non-negative integers. For any two tuples $\alpha = (\alpha_1, \alpha_2)$, $l = (l_1, l_2) \in N^2$, $|\alpha| = \alpha_1 + \alpha_2$, $|l|_\infty = \max(|l_1|, |l_2|)$. Throughout this paper, we denote by c a generic positive constant independent of any function. The Legendre polynomial of degree l is defined by

$$L_l(x) = L_{l_1}(x_1)L_{l_2}(x_2), \tag{1}$$

where

$$L_{l_q}(x_q) = \frac{(-1)^{l_q}}{2^{l_q} l_q!}\partial_{x_q}^{l_q}(1-x_q^2)^{l_q}, q = 1,2. \tag{2}$$

The set of Legendre polynomials is a L^2-orthogonal system on Ω, i.e.,

$$\int_\Omega L_l(x)L_k(x)dx = \left(l_1 + \frac{1}{2}\right)^{-1}\left(l_2 + \frac{1}{2}\right)^{-1}\delta_{l,k} \tag{3}$$

where $\delta_{l,k}$ is the Kronecher symbol.

For any $v \in L^2(\Omega)$, we may write $v(x) = \sum_{|l|_\infty = 0}^\infty \hat{v} L_l(x)$, where

$$\hat{v}_l = \left(l_1 + \frac{1}{2}\right)\left(l_2 + \frac{1}{2}\right)\int_\Omega v(x)L_l(x)dx, |l| = 0,1,\ldots. \tag{4}$$

We first recall some properties of the Legendre approximation. Let N be any positive integer and B_N be the set of all algebraic polynomials of degree at most N in each variable. We turn to the inverse inequalities in the space B_N.

Lemma 1[24] Let n be an non-negative integer and $|\alpha| = n$, then for any $\phi \in P_N$,

$$\|D^\alpha \phi\| \le cN^{2n}\|\phi\|. \tag{5}$$

Also for any $r \ge 0$,

$$\|\phi\|_r \le cN^{2r}\|\phi\|. \tag{6}$$

The L^2 − orthogonal projection of a function $v \in L^2(\Omega)$ is

$$P_N v(x) = \sum_{|l|_\infty = 0}^N \hat{v}_l L_l(x) \cdot \tag{7}$$

Lemma 2 [24] If $r \ge 0$, then for any $v \in H^r(\Omega)$

$$\|v - P_N v\| \le cN^{-r}\|v\|_r. \tag{8}$$

We now turn to the discrete Legendre approximation. Let $x^{(j)} = (x_1^{(j_1)}, x_2^{(j_2)})$, $0 \le j_q \le N$, $\{x_q^{(k)}\}_{k=0}^N$ are LGL points [24] and

$$\omega_{j_q} = \frac{2}{N(N+1)}\frac{1}{[L_N(x_q^{(j_q)})]^2}, 0 \le j_q \le N. \tag{9}$$

Let Ω_N be the set of all $x^{(j)}$. We can define discrete inner product in $C(\overline{\Omega})$ and its associated norm by

$$\langle u, v\rangle_{N,\omega} = \sum_{j_1=0}^N \sum_{j_2=0}^N u(x^{(j)})v(x^{(j)})\omega_{j_1}\omega_{j_2}$$

$$\|u\|_{N,\omega} = \langle u, u\rangle_{N,\omega}^{\frac{1}{2}} \tag{10}$$

We have

$$\langle L_l, L_k\rangle_{N,\omega} = \begin{cases} 0 & , \quad l \ne k \\ \dfrac{2}{N} & , \quad l = k. \end{cases} \tag{11}$$

Lemma 3 [24] $\quad \|u\| \le \|u\|_{N,\omega} \le \sqrt{3}\|u\|$ (12)

The Legendre interpolation $I_N v(x) \in B_N$ of a function $v \in C(\overline{\Omega})$ is defined by

$$I_N v(x^{(j)}) = v(x^{(j)}), \forall x^{(j)} \in \Omega_N. \tag{13}$$

Lemma 4 [24] If $v \in H^r(\Omega)$, $r > \frac{1}{2}$, then

$$\|v - I_N v\| \le cN^{-r}\|v\|_r. \tag{14}$$

3.A mollification method by using Legendre expansion

We will discuss the following problem. Suppose that we know an approximate function $g^\delta \in L^2(\Omega)$ of $g \in H^r(\Omega)$ such that

$$\|g^\delta - g\| \le \delta, \|g^\delta\| \ge \tau\delta \tag{15}$$

where $\delta > 0$ is a given constant called the error level and $\tau > 1$. We want to approximate $D^\alpha g$ from g^δ. Our idea is to compute approximate derivatives with the following mollification method. At first, we mollify g^δ by using the projection operator

$$g^\delta \to f_{n,\delta} = P_n g^\delta = \sum_{l=0}^{n} \hat{g}_l^\delta L_l(x). \tag{16}$$

The mollification parameter n plays an essential role in the accuracy of these approximations. In this paper, we make use of a discrepancy principle to obtain an optimal an a posteriori chosen $n(\delta, g^\delta)$:

$$\left\|(I-P_n)g^\delta\right\| \le \tau\delta < \left\|(I-P_{n-1})g^\delta\right\|. \tag{17}$$

Then $D^\alpha f_{n,\delta}$ will be used as an approximation of $D^\alpha g$, we will prove a convergence estimate in the following.

Theorem 5 Suppose that $f_{n,\delta}$ is defined by (16) and (17), $g \in H^r(\Omega)$, then for any $|\alpha| \le \frac{r}{2}$, we have

$$\left\|D^\alpha f_{n,\delta} - D^\alpha g\right\| = O(\delta^{\frac{r-2|\alpha|}{r}}).$$

(18)

Proof: By Lemma 1 and 2

$$\begin{aligned} \left\|f_{n,\delta} - g\right\|_{r/2} &= \left\|P_n(g^\delta - g) + P_n g - g\right\|_{r/2} \\ &\le \left\|P_n(g^\delta - g)\right\|_{r/2} + \left\|P_n g - g\right\|_{r/2} \\ &\le cn^r + cn^{-r/2}\left\|g\right\|_{r/2} \end{aligned} \tag{19}$$

On the other hand

$$\begin{aligned} \left\|P_{n-1}g - g\right\| &= \left\|(P_{n-1}g^\delta - g^\delta) - (I-P_{n-1})(g-g^\delta)\right\| \\ &\ge \left\|P_{n-1}g^\delta - g^\delta\right\| - \left\|(I-P_{n-1})(g-g^\delta)\right\|. \end{aligned} \tag{20}$$

From (17), we have

$$\left\|P_{n-1}g^\delta - g\right\| \ge \tau\delta. \tag{21}$$

And

$$\left\|(I-P_{n-1})(g^\delta - g)\right\| \le \left\|g^\delta - g\right\| \le \delta. \tag{22}$$

Hence

$$\left\|P_{n-1}g - g\right\| \ge (\tau-1)\delta. \tag{23}$$

From Lemma 2, we can obtain

$$(\tau-1)\delta \le \left\|P_{n-1}g - g\right\| \le c(n-1)^{-r}\left\|g\right\|_r \tag{24}$$

Thus we can get

$$m \le \left(\frac{c\left\|g\right\|_r}{\tau-1}\right)^{\frac{1}{r}} \delta^{-\frac{1}{r}} + 1 \tag{25}$$

So by (19), there exists a constant M which does not depend on δ such that

$$\left\|f_{n,\delta} - g\right\|_{r/2} \le M. \tag{26}$$

Moreover,

$$\left\|f_{n,\delta} - g\right\| \le \left\|f_{n,\delta} - g^\delta\right\| + \left\|g^\delta - g\right\| \le (\tau+1)\delta. \tag{27}$$

The assertion of theorem will be obtained by interpolation [23].

$$\left\|u\right\|_\mu \le K \left\|u\right\|_{r/2}^{\frac{\mu}{r/2}} \left\|u\right\|^{\frac{r/2-\mu}{r/2}}, \mu \le r, \forall u \in H^{r/2}(\Omega). \tag{28}$$

4.A mollification method by using LGL interpolation

In this section, we derive corresponding results for pseudo-spectral approximations which are more convenient in actual computations. In practical, the perturbed data are usually given at nodes. Suppose that the data is given at points $x^{(j)} \in \Omega_N$, such that

$$|g^\delta(x^{(j)}) - g(x^{(j)})| \le \delta_1. \tag{29}$$

We can obtain the following Lemma

Lemma 6. Suppose that the perturbed data $g^\delta(x^{(j)})$ satisfies (29), then we have

$$\left\|I_N g^\delta - I_N g\right\|_{N,\omega} \le 2\delta_1 =: \hat{\delta}.$$

(30)

Proof:

$$\begin{aligned} \left\|I_N g^\delta - I_N g\right\|_{N,\omega} &= \left(\sum_{j_1=0}^{N}\sum_{j_2=0}^{N}(g^\delta(x^{(j)}) - g(x^{(j)}))^2 \omega_{j_1}\omega_{j_2}\right)^{1/2} \\ &\le \delta_1\left(\sum_{j_1=0}^{N}\sum_{j_2=0}^{N}\omega_{j_1}\omega_{j_2}\right)^{1/2} \\ &= 2\delta_1 \end{aligned} \tag{31}$$

Using the LGL interpolation, we can give the approximate function as follows:

$$\mathrm{f}_\delta = \mathrm{f}_{n_1,\delta}(x) = P_{n_1} I_N g^\delta. \tag{32}$$

where n_1 is determined by the discrepancy principle

$$\left\|(I-P_{n_1})I_N g^\delta\right\|_N \le \tau\delta < \left\|(I-P_{n_1-1})I_N g^\delta\right\|_N \tag{33}$$

with $\tau > 1$.

We now state the main result of this section.

Theorem 7. Suppose that $\mathrm{f}_{n_1,\delta}$ is defined by (32) and (33), $g \in H^r(\Omega)$, then for any $|\alpha| \le \frac{r}{2}$, we have

$$\left\|D^\alpha \mathrm{f}_{n,\delta} - D^\alpha g\right\| = O(\hat{\delta}^{\frac{r-2|\alpha|}{r}} + N^{2|\alpha|-r}). \tag{34}$$

Proof: By Lemma 1 and 2

$$\begin{aligned} \left\|\mathrm{f}_{n_1,\delta} - g\right\|_{r/2} &= \left\|P_{n_1}(I_N g^\delta - I_N g) + P_{n_1}I_N g - I_N g + I_N g - g\right\|_{r/2} \\ &\le \left\|P_{n_1}(I_N g^\delta - I_N g)\right\|_{r/2} + \left\|P_{n_1}I_N g - I_N g\right\|_{r/2} + \left\|I_N g - g\right\|_{r/2} \\ &\le cn^r + cn^{-r/2}\left\|g\right\|_{r/2} \end{aligned} \tag{35}$$

From (33), we have

$$\left\|P_{n_1-1}I_N g^\delta - I_N g^\delta\right\|_{N,\omega} \ge \tau\hat{\delta} \tag{36}$$

and

$$\left\|(I-P_{n_1-1})(I_N g^\delta - I_N g)\right\|_{N,\omega} \le \hat{\delta}. \tag{37}$$

Hence

$$\left\|P_{n_1-1}I_N g - I_N g\right\|_{N,\omega} \ge (\tau-1)\hat{\delta}. \tag{38}$$

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From Lemma 2 and 3, we can obtain

$$\begin{aligned}
(\tau-1)\hat{\delta} &\le \left\|P_{n_1-1}I_N g - I_N g\right\|_{N,\omega} \\
&\le \sqrt{3}\left\|P_{n_1-1}I_N g - I_N g\right\| \\
&= \sqrt{3}\left\|P_{n_1-1}I_N g - P_{n_1} g + P_{n_1} g - g + g - I_N g\right\| \\
&\le 2\sqrt{3}\left\|I_N g - g\right\| + \left\|P_{n_1} g - g\right\| \\
&\le 2\sqrt{3}\left\|I_N g - g\right\| + \left\|P_{n_1} g - g\right\| \\
&\le 2\sqrt{3}cN^{-r}\left\|g\right\|_r + c(n_1-1)^{-r}\left\|g\right\|_r
\end{aligned} \tag{39}$$

Thus we can get

$$n_1 \le \left(\frac{C\|g\|_r}{\tau-1}\right)^{1/r}\hat{\delta}^{-1/r}. \tag{40}$$

By (35), there exists a constant M_1 such that

$$\left\|f_{n_1,\delta} - g\right\|_{r/2} \le M_1. \tag{41}$$

Moreover,

$$\begin{aligned}
\left\|f_{n_1,\delta} - g\right\| &\le \left\|f_{n_1,\delta} - I_N g^{\delta}\right\| + \left\|I_N g^{\delta} - I_N g\right\| + \left\|I_N g - g\right\| \\
&\le \left\|f_{n_1,\delta} - I_N g^{\delta}\right\|_{N,\omega} + \left\|I_N g^{\delta} - I_N g\right\|_{N,\omega} + cN^{-r}\left\|g\right\| \\
&\le (\tau+1)\hat{\delta} + cN^{-r}\left\|g\right\|
\end{aligned} \tag{42}$$

The assertion of theorem will be obtained by interpolation inequality [23]

$$\|u\|_{\mu} \le K\|u\|_{r/2}^{\frac{\mu}{r/2}}\|u\|^{\frac{r/2-\mu}{r/2}}, \mu \le r, \forall u \in H^{r/2}(\Omega).$$

(43)

5. Numerical examples

We provide numerical examples in this section. Let $g(x)$ be a function with two variables given by

$$g(x) = \cos(\pi x_1)\sin(\pi x_2), x \in \Omega.$$

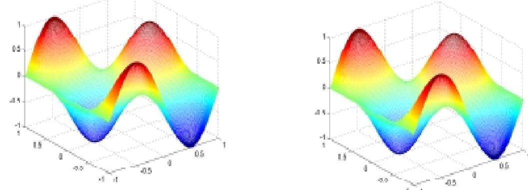

Figure 1: Functions g and its approximation

The discretization knots are $x^{(j)} \in \Omega_N$. The perturbed discrete data are given by

$$g^{\delta}(x^{(j)}) = g(x^{(j)}) + \varepsilon_j, |\varepsilon_j| \le \overline{\delta},$$

where $\{\varepsilon_j\}_{j=1}^{(N+1)^2}$ are generated by Function $2\times(\mathrm{rand}(N+1)-1)\times\overline{\delta}$ in Matlab. The numerical results of constructing g, g_{x_1} g_{x_2} $g_{x_1x_1}$ $g_{x_1x_2}$ $g_{x_2x_2}$ with N=256, $\overline{\delta}$=0.01 are illustrated in Figs. 1-6., respectively. In Figs. 1-6, the left figures are the original functions and the right figures are the constructed functions. In Figs. 7-9, the constructed errors of g, g_{x_1} g_{x_2} $g_{x_1x_1}$ $g_{x_1x_2}$ $g_{x_2x_2}$ are presented, respectively. In Figs. 1-6, we observe that the reconstructed functions are very similar to those of the corresponding functions. In the following, we also further investigate how the relative errors depend on δ.

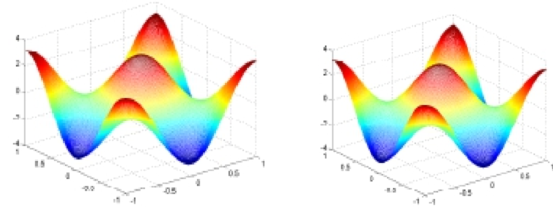

Figure 2: Functions g_{x_1} and its approximation

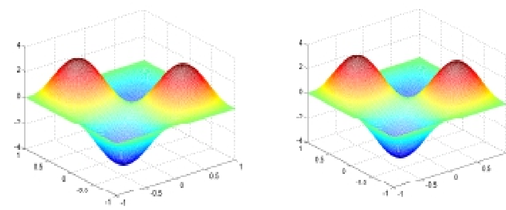

Figure 3: Functions g_{x_2} and its approximation

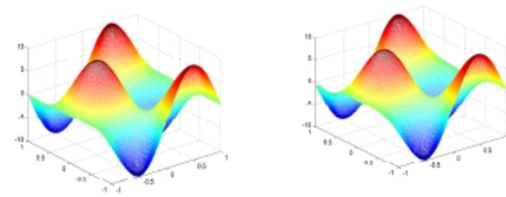

Figure 4: Functions $g_{x_1x_1}$ and its approximation

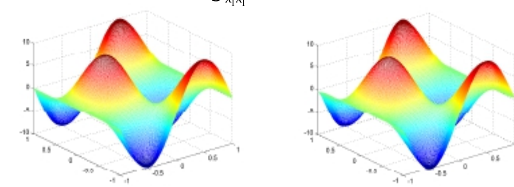

Figure 5: Functions $g_{x_2x_2}$ and its approximation

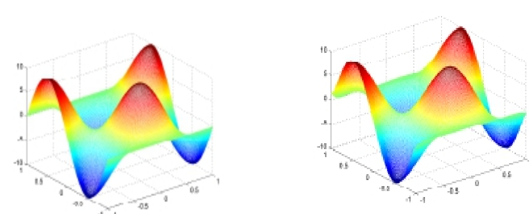

Figure 6: Functions $g_{x_1x_2}$ and its approximation

The relative errors $\varepsilon_g, \varepsilon_{g_{x_1}}, \varepsilon_{g_{x_2}}, \varepsilon_{g_{x_1x_1}}, \varepsilon_{g_{x_2x_2}}$, $\varepsilon_{g_{x_1x_2}}$ are presented in Table 1 when $\overline{\delta}$ increases form 0.0001 to 0.1 with fixed *N*=256. Here, the relative error ε_g are defined as

$$\varepsilon_g = \frac{\left\| f_{n_1,\delta} - g \right\|_{N,\omega}}{\left\| g \right\|_{N,\omega}}.$$

We also defined $\varepsilon_{g_{x_1}}, \varepsilon_{g_{x_2}}, \varepsilon_{g_{x_1x_1}}, \varepsilon_{g_{x_2x_2}}, \varepsilon_{g_{x_1x_2}}$, in the same way.

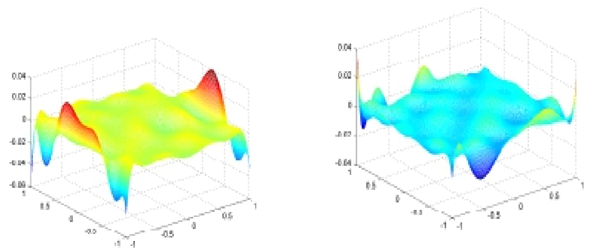

Figure 7: Constructed errors of g_{x_1} and g_{x_2}

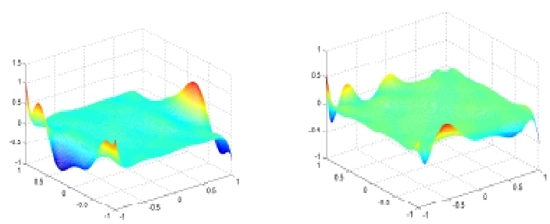

Figure 8: Constructed errors of $g_{x_1x_1}$ and $g_{x_2x_2}$

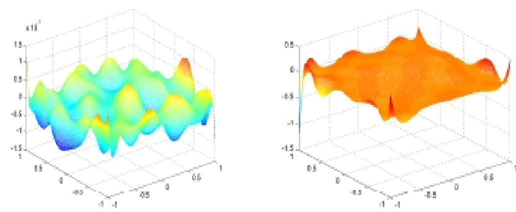

Figure 9: Constructed errors of g and $g_{x_1x_2}$

From Table 1, we can see that when the noise level $\overline{\delta}$ is decreased from 0.1 to 0.0001, the relative errors will decrease too. The above numerical results show that the proposed method is efficient.

6. Conclusion

In this paper, we proposed a new mollification method to reconstruct numerical derivatives from noisy data. The theoretical analyses show that the smoother the genuine solution, the higher the convergence rates of the numerical solution by our methods. Especially if $g \in H^{\infty}(\Omega)$, then the convergence rates of numerical derivatives is $O(\delta)$. Moreover, the solution processes will be uniform for different derivatives, which means that the method is self-adaptive. All the test numerical examples presented in the paper show that the new method works well. The extension of the work to piecewise smooth function is now under investigation.

Table 1: Relative errors with different noise level

$\overline{\delta}$	1e-1	1e-2	1e-3	1e-4
ε_g	3.7147e-3	4.4912e-4	5.7346e-5	5.3339e-6
$\varepsilon_{g_{x_1}}$	1.0487e-2	2.4506e-3	1.7774e-4	2.1542e-5
$\varepsilon_{g_{x_2}}$	1.3426e-2	1.4016e-3	4.2203e-4	3.3407e-5
$\varepsilon_{g_{x_1x_1}}$	4.6777e-2	1.8234e-2	1.3249e-3	1.7913e-4
$\varepsilon_{g_{x_1x_2}}$	7.0255e-2	8.0529e-3	3.9971e-3	3.7298e-4
$\varepsilon_{g_{x_2x_2}}$	2.9172e-2	5.5944e-3	8.7607e-4	1.3671e-4

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