UTMS 2002–14 March 20, 2002

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Abstract. In this paper, we discuss a classical ill-posed problem– numerical differentiation by the Tikhonov regularization. Based on the conditional stability estimate for this ill-posed problem, a new simple method for choosing regularization parameters is proposed. We show that it has an almost optimal convergence rate when the exact solution is in H^2. The advantages of our method are: 1. We can get a similar computational results with much less computation, in comparison with other methods; 2. We can find out the discontinuous points numerically.

1. Introduction

A numerical differentiation problem, which is determination of the derivative of the function from values at discrete points, is important in the scientific research and practical applications. This problem arise from many mathematical models and practical problems, for example, the identification of the discontinuous points in an image process([3]); the problems of solving the Abel integral equation([6]); the problems of determining the peaks in spectroscopy of chemistry([11]) and some inverse problem in mathematical physical equation ([10]), etc. The main difficulty is that it is an ill-posed problem. This means that every small error in the measurement may cause huge errors in the numerical results ([7], [10],[20]). For the numerical differentiation problem, there are works concerning the convergence analysis of the numerical algorithms (e.g. [8],[10], [15], etc.). One of their method is to use a finite difference to approximate the derivatives and suitably choose the

Date: March 20, 2002.

1991 *Mathematics Subject Classification.* 65D25, 45D05, 35R25.

Key words and phrases. Numerical differentiation, Tikhonov regularization, discontinuous point.

This work is partially support by NSF of China (19971016) and the Laboratory of Nonlinear Sciences in Fudan University, Shanghai, China.

size of mesh. It has been shown that, if the data contains some errors, then the size of the mesh should not be too small, or in other words, the number of the measuring points should not be too big. Otherwise the errors of the approximation solutions may be very large. Another way for treating the numerical differentiation problem is to use the Tikhonov regularization which has been shown quite effective for ill-posed problems and inverse problems ([4], [7], [12]). Recently, Hanke and Scherzer provided a very effective analysis for treating the numerical differentiation problem by the Tikhonov regularization([10]). The error estimate is also proved in their paper. Motivated by their way and results, we also consider the numerical differentiation problem by the Tikhonov regularization. The differences between our results and the results in [10] are:

(1). We consider the numerical differentiation problem on a irregular grid which is different from [10].

(2). We use a very simple strategy of choosing the regularization parameter which is different from Discrepancy Principle used in [10]. We can also prove the similar error estimates as [10]. It can be shown that we can get similar numerical results with much less computational time. The idea of this choosing strategy comes from the results in [2] which is based on the conditional stability for the inverse and ill-posed problems.

(3). We also consider the case that the exact solution has not enough regularity.

We show that the properties of the regularized solution can be used to determine the discontinuous points of the exact solution.

The paper is organized as follows: In Section 2, we give the formulation of the problem and our main theoretic results. In Section 3, we prove them. Some numerical examples and applications are presented in Section 4. Finally, we give some remarks in Section 5.

2. Formulation of the problem and the main results

Suppose that $y = y(x)$ is a function on [0,1], n is a natural number and $\Delta = \{0 = x_0 < x_1 < \cdots < x_n = 1\}$ is a grid of $[0, 1]$. Let δ be a given constant which we call the level of noise in the data.

We denote

$$h_i = x_{i+1} - x_i, \qquad i = 0, 1, \cdots, n-1,$$

$$h = \max_{0 \le i \le n-1} h_i.$$

We consider the following numerical differentiation problem:

Given the noisy samples $\widetilde{y}_i$ of the values $y(x_i)$ which satisfy

$$|\widetilde{y}_i - y(x_i)| \le \delta, \qquad i = 1, 2, \cdots, n,$$

we want to find a function $f_*(x)$ so that $f_*^{'}(x)$ can be an approximation of the function $y^{'}(x)$.

Here $'$ denotes the derivative with respect to x.

Without lose of the generality, we can assume that $\widetilde{y}_0 = y(0)$, $\widetilde{y}_n = y(1)$. Otherwise we can use a new function

$$Y(x) = y(x) + \widetilde{y}_0 - y(0) + (\widetilde{y}_n - y(1) + y(0) - \widetilde{y}_0)x$$

to replace $y(x)$. It can be easily proved that $Y(0) = \widetilde{y}_0$, $Y(1) = \widetilde{y}_n$ ([10]).

We recall the definitions of the usual spaces:

$$L^2(0,1) = \left\{ g \,|\, (\int_0^1 g^2(x)dx)^{1/2} < \infty \right\},$$

$$H^k(0,1) = \left\{ g \,|\, g \in L^2(0,1),\, g^{(k)} \in L^2(0,1) \right\},$$

$$C[0,1] = \{ g \,|\, g \text{ is a continuous function on } [0,1] \}$$

The norms of these spaces are defined as

$$\|g\|_{L^2(0,1)} = \left(\int_0^1 |g(x)|^2 dx \right)^{1/2},$$

$$\|g\|_{H^k(0,1)} = \left(\|g\|^2_{L^2(0,1)} + \left\| g^{(k)} \right\|^2_{L^2(0,1)} \right)^{\frac{1}{2}}$$

$$\|g\|_{C[0,1]} = \max_{x \in [0,1]} |g(x)|$$

Here $^{(k)}$ denotes the k-th order derivative with respect to x.

We define a cost functional:

$$\Phi(f) = \sum_{j=1}^{n-1} \frac{h_i + h_{i+1}}{2} (\widetilde{y}_j - f(x_j))^2 + \alpha \left\| f^{''} \right\|^2_{L^2(0,1)} \tag{2.1}$$

where α is a regularization parameter.

We can discuss the following two problems:

Problem 1: Find $f_* \in H^2(0,1)$ which satisfies $f_*(0) = y(0)$, $f_*(1) = y(1)$ such that

$$\Phi(f_*) \leq \Phi(f), \tag{2.2}$$

for all $f \in H^2(0,1)$ with $f(0) = y(0)$, $f(1) = y(1)$.

If such f_* exists, we consider

Problem 2: How to choose the regularization parameter α, which is related to δ, so that $f_*^{'}(x)$ can be an approximation of $y^{'}(x)$?

Remark 2.1. It is well known that the choice of the regularization parameter is very important. In [10], the author used a way called the discrepancy principle.

Remark 2.2. From the results in [2], we know that the conditional stability implies the convergence rate of the Tikhonov regularizing solution. It can be shown that the process of differentiation is conditional stable in the sense of that, for $f \in H^2(0,1)$, and $f(0) = 0$, $f(1) = 0$, it holds

$$\left\| f^{'} \right\|_{L^2(0,1)}^2 \leq \|f\|_{L^2(0,1)} \left\| f^{''} \right\|_{L^2(0,1)}.$$

Therefore it is possible to apply the way in [2] to our problem.

We have the following theoretic results:

Theorem 2.3. *There exists a unique solution f_* of the Problem 1. Later we will give an algorithm for construction of f_*.*

Theorem 2.4. *Suppose that f_* is the solution of Problem 1. We take $\alpha = \delta^2$. If $y \in H^2(0,1)$, then we have*

$$\left\| f_*^{'} - y^{'} \right\|_{L^2(0,1)} \leq (2h + 4\sqrt{\delta} + \frac{h}{\pi}) \left\| y^{''} \right\|_{L^2(0,1)} + h + 2\sqrt{\delta} \tag{2.3}$$

Theorem 2.5. *Suppose that f_* is the minimizer solution of Problem 1. We take $\alpha = \delta^2$. If $y \in C[0,1] \setminus H^2(0,1)$, then we have*

$$\left\| f_*^{''} \right\|_{L^2(0,1)} \longrightarrow \infty, \qquad as \quad \delta, h \to 0.$$

Remark 2.6. For a piecewise continuous function, the conclusions in Theorem2.5 is still true. We can prove it by the small modification of our proof. In fact, we can prove that, if x_0 is a discontinuous point of $y(x)$, then, for every open interval I_1 which contains x_0, $\left\| f_*^{''} \right\|_{L^2(I_1)} \to \infty$ as $h \to 0$ and $\delta \to 0$.

Remark 2.7. In Theorem 2.5, we discuss the case of the exact solution $y \in C[0,1] \setminus H^2(0,1)$. This result can be used in order to determine a discontinuous point from the values of the function on some discrete points. We give one application in Section 4.

3. Proofs of the theoretic results

3.1. **Preliminary.** Before the proofs we first state several known results concerning the spline and interpolations.

Definition 1. We call a function $h(x)$ the natural cubic spline on $[0,1]$, if it is continuously twice differentiable on $[0,1]$ and

(1) $h(x)$ is a cubic polynomial on $[x_i, x_{i+1}]$; $0 \le i \le n-1$.
(2) $h^{''}(0) = h^{''}(1) = 0$.

Lemma 3.1. *Suppose that* y *is a smooth function on* $(0,1)$ *and* s *is a natural cubic spline of the grid* Δ *such that* $s(x_i) = y(x_i), i = 0, 1, \cdots, n$, *then we have*

$$\left\| s^{''} - y^{''} \right\|^2_{L^2(0,1)} + \left\| s^{''} \right\|^2_{L^2(0,1)} = \left\| y^{''} \right\|^2_{L^2(0,1)} \tag{3.1}$$

This result can be found in [9], [5].

Lemma 3.2. *Suppose that* y *is a smooth function on* $(0,1)$ *and* s *is a natural cubic spline of the grid* Δ *such that* $s(x_i) = y(x_i), i = 0, 1, \cdots, n$, *then we have*

$$\left\| s^{'} - y^{'} \right\|_{L^2(0,1)} \le \frac{h}{\pi} \left\| y^{''} \right\|_{L^2(0,1)} \tag{3.2}$$

where $h = max\{h_i\}$.

The result can be found in [19].

Lemma 3.3. *Let* $g \in H^2(0,1)$. *We define a piecewise constant function* χ *by*

$$\chi|_(x_{i-1}, x_i) = \chi_i = \frac{1}{h_{i-1}} \int_{x_{i-1}}^{x_i} g(x)dx,$$

then we have

$$\| g - \chi \|_{L^2(0,1)} \le h \left\| g^{'} \right\|_{L^2(0,1)}. \tag{3.3}$$

This result can be found in [17].

Remark 3.4. In most references, these results are stated and proved in the case that the grid Δ is uniform. It can be easily proved that the result is still true when the grid is not uniform.

3.2. **Proof of theorem 2.3.** We will prove this theorem in two steps:

Step 1: Construct f_*

f_* can be constructed by the following way:

1. f_* is a twice differentiable natural cubic spline of grid Δ. That is

$$\begin{aligned} f_*(x_i+) &= f_*(x_i-), & f_*^{'}(x_i+) &= f_*^{'}(x_i-), \\ f_*^{''}(x_i+) &= f_*^{''}(x_i-), & i &= 1,2,\cdots,n-1. \end{aligned}$$

where $f_*(x_i+) = \lim_{x\to x_i+} f(x)$, $f_*(x_i-) = \lim_{x\to x_i-} f(x)$.

2. $f_*^{''}(0) = f_*^{''}(1) = 0$.

3. At x_i, $i = 1,2,\cdots,n-1$, the third order derivative of f_* satisfies the following condition:

$$f_*^{'''}(x_i+) - f_*^{'''}(x_i-) = \frac{1}{\delta^2}\frac{h_i + h_{i+1}}{2}(\widetilde{y}_i - f_*(x_i)), \qquad i = 1,2,\cdots,n-1. \tag{3.4}$$

See [16], [18] for the detail of the construction of f_*.

Step 2: Prove that f_* is a unique minimizer of the function Φ.

First, it is easily proved that,

Lemma 3.5. *Suppose that $g \in H^2(0,1)$ and $g(0) = g(1) = 0$, then we have*

$$\int_0^1 g^{''} f_*^{''} dx = \frac{1}{\delta^2(n-1)} \sum_{i=1}^{n-1} (g(x_i)(\widetilde{y}_i - f_*(x_i))). \tag{3.5}$$

Next, by using (2.1) and Lemma 3.5, we have

$$\begin{aligned} \Phi(f) - \Phi(f_*) &= \sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2}(f(x_i) - f_*(x_i))(f(x_i) + f_*(x_i) - 2\widetilde{y}_i) \\ &\quad + \delta^2 \left\| f^{''} - f_*^{''} \right\|^2_{L^2(0,1)} + 2\delta^2 \int_0^1 (f^{''} - f_*^{''}) f_*^{''} dx \\ &= \sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2}(f(x_i) - f_*(x_i))(f(x_i) + f_*(x_i) - 2\widetilde{y}_i) \\ &\quad + 2\sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2}(f(x_i) - f_*(x_i))(\widetilde{y}_i - f_*(x_i)) \\ &\quad + \delta^2 \left\| f^{''} - f_*^{''} \right\|^2_{L^2(0,1)}. \end{aligned}$$

Therefore, we have

$$\Phi(f)-\Phi(f_*)=\sum_{i=1}^{n-1}\frac{h_i+h_{i+1}}{2}(f(x_i)-f_*(x_i))^2+\delta^2\left\|f^{''}-f_*^{''}\right\|_{L^2(0,1)}^2\geq 0 \tag{3.6}$$

This shows that f_* is the minimizer of Φ.

Furthermore, we assume that there exists another function $f\in H^2(0,1)$ which satisfies $f(0)=y(0)$, $f(1)=y(1)$, and $\Phi(f)=\Phi(f_*)$. Then, by (3.6), we have

$$\left\|f^{''}-f_*^{''}\right\|_{L^2(0,1)}^2=0,\qquad f(x_i)=f_*(x_i),\quad i=1,2,\cdots,n-1.$$

Hence

$$f^{''}=f_*^{''}.$$

That is

$$f-f_*=ax+b.$$

Since $f(0)=f_*(0)$, $f(1)=f_*(1)$, we have that

$$f=f_*.$$

The proof is completed.

3.3. **Proof of Theorem 2.4.** Suppose that s is a natural cubic spline which interpolates the exact data $y(x_i), i=0,\cdots,n$. We denotes $e(x)=f_*(x)-s(x)$. It is obvious that $e(1)=e(0)=0$.

We define a piecewise constant function $\chi(x)\in L^2(0,1)$:

$$\chi(x)=\frac{e(x_i)-e(x_{i-1})}{h_{i-1}}=\chi_i,\qquad x\in(x_{i-1},x_i),\qquad i=1,2,\cdots,n-1. \tag{3.7}$$

By (3.7), we can have

$$\begin{aligned}\left\|e^{'}\right\|_{L^2(0,1)}^2 &= \int_0^1(e^{'}(x))^2dx=\int_0^1 e^{'}(e^{'}-\chi)dx+\int_0^1 e^{'}\chi dx\\ &= \int_0^1 e^{'}(e^{'}-\chi)dx+\sum_{i=1}^{n-1}\chi_i(e(x_i)-e(x_{i-1}))\\ &= \int_0^1 e^{'}(e^{'}-\chi)dx+\sum_{i=1}^{n-1}e(x_i)(\chi_i-\chi_{i+1})\\ &= I_1+I_2 \qquad (3.8)\end{aligned}$$

It remains to estimate the two terms I_1 and I_2 in (3.8).

From the expression of I_1 and Lemma 3.3, we obtain

$$I_1 \leq \left\|e^{'}\right\|_{L^2(0,1)} \left\|e^{'} - \chi\right\|_{L^2(0,1)} \leq h \left\|e^{'}\right\|_{L^2(0,1)} \left\|e^{''}\right\|_{L^2(0,1)}.$$

Since f_* is the minimizer of Φ, it can be verified that

$$\begin{aligned} \delta^2 \left\|f_*^{''}\right\|_{L^2(0,1)} &\leq \Phi(f_*) \leq \Phi(y) \\ &= \sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2} (\widetilde{y}_i - y(x_i))^2 + \delta^2 \left\|y^{''}\right\|^2_{L^2(0,1)} \\ &\leq \delta^2 + \delta^2 \left\|y^{''}\right\|^2_{L^2(0,1)} = \delta^2 (1 + \left\|y^{''}\right\|^2_{L^2(0,1)}). \end{aligned} \tag{3.9}$$

Therefore we have

$$\left\|f_*^{''}\right\|^2_{L^2(0,1)} \leq 1 + \left\|y^{''}\right\|^2_{L^2(0,1)}.$$

Hence

$$\begin{aligned} \left\|e^{''}\right\|_{L^2(0,1)} &= \left\|f_*^{''} - s^{''}\right\|_{L^2(0,1)} \\ &\leq \left\|f_*^{''}\right\|_{L^2(0,1)} + \left\|s^{''}\right\|_{L^2(0,1)} \\ &\leq \left(1 + \left\|y^{''}\right\|^2_{L^2(0,1)}\right)^{\frac{1}{2}} + \left\|y^{''}\right\|_{L^2(0,1)} \\ &\leq 1 + 2\left\|y^{''}\right\|_{L^2(0,1)}. \end{aligned}$$

Finally, we have

$$I_1 \leq h \left\|e^{'}\right\|_{L^2(0,1)} \left(1 + 2\left\|y^{''}\right\|_{L^2(0,1)}\right).$$

We apply Cauchy-Schwartz inequality to I_2

$$\begin{aligned} I_2^2 &= \left(\sum_{i=1}^{n-1} \left(\frac{h_i + h_{i+1}}{2}\right)^{\frac{1}{2}} e(x_i) \left(\frac{2}{h_i + h_{i+1}}\right)^{\frac{1}{2}} (\chi_i - \chi_{i+1}) \right)^2 \\ &\leq \left(\sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2} e^2(x_i) \right) \left(\sum_{i=1}^{n-1} \frac{2}{h_i + h_{i+1}} (\chi_i - \chi_{i+1})^2 \right) \end{aligned}$$

By the definition of χ, we have

$$\begin{aligned}
\chi_i - \chi_{i+1} &= \frac{1}{h_i}\int_{x_{i-1}}^{x_i} e^{'}(x)dx - \frac{1}{h_{i+1}}\int_{x_i}^{x_{i+1}} e^{'}(x)dx \\
&= \frac{x_i - x_{i-1}}{h_i}\int_0^1 e^{'}(h_i\tau + x_{i-1})d\tau \\
&\quad -\frac{x_{i+1} - x_i}{h_{i+1}}\int_0^1 e^{'}(h_{i+1}\tau + x_i)d\tau \\
&= \int_0^1 (e^{'}(h_i\tau + x_{i-1}) - e^{'}(h_{i+1}\tau + x_i))d\tau \\
&= \int_0^1 \int_{h_{i+1}\tau+x_i}^{h_i\tau+x_{i-1}} e^{''}(x)dxd\tau.
\end{aligned}$$

Therefore we can get

$$\begin{aligned}
|\chi_i - \chi_{i+1}| &\le \int_0^1 \int_{x_{i-1}}^{x_{i+1}} \mid e''(x) \mid dxd\tau \\
&\le (x_{i+1} - x_{i-1}) \left\| e^{''} \right\|_{L^2(0,1)} \\
&= (h_i + h_{i+1}) \left\| e^{''} \right\|_{L^2(0,1)}.
\end{aligned}$$

Since f_* is the unique minimizer of Φ, we have

$$\begin{aligned}
&\sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2}(f_*(x_i) - \widetilde{y}_i)^2 \le \Phi(y) \\
&\le \left(\delta^2 + \delta^2 \left\| y^{''} \right\|_{L^2(0,1)}^2\right).
\end{aligned}$$

By the assumptions on $\widetilde{y}_i$, it is easy to verify that

$$\sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2}(y(x_i) - \widetilde{y}_i)^2 \le \delta^2.$$

Therefore, we have

$$\begin{aligned}\sum_{i=1}^{n-1}\frac{h_i+h_{i+1}}{2}e^2(x_i) &= \sum_{i=1}^{n-1}\frac{h_i+h_{i+1}}{2}(f_*(x_i)-y(x_i))^2\\ &\le \sum_{i=1}^{n-1}(h_i+h_{i+1})((f_*(x_i)-\widetilde{y}_i)^2+(\widetilde{y}_i-y(x_i))^2\\ &\le 2\Phi(y)+2\sum_{i=1}^{n-1}\frac{h_i+h_{i+1}}{2}(\widetilde{y}_i-y(x_i))^2\\ &\le 2\delta^2\left(1+\left\|y^{''}\right\|^2_{L^2(0,1)}\right)+2\delta^2\\ &\le 2\delta^2\left(2+\left\|y^{''}\right\|^2_{L^2(0,1)}\right).\end{aligned}$$

Hence

$$\begin{aligned}I_2^2 &\le \left(\sum_{i=1}^{n-1}\frac{h_i+h_{i+1}}{2}e^2(x_i)\right)\left(\sum_{i=1}^{n-1}2(h_i+h_{i+1})\left\|e^{''}\right\|^2_{L^2(0,1)}\right)\\ &\le 2\delta^2\left(2+\left\|y^{''}\right\|^2_{L^2(0,1)}\right)\sum_{i=1}^{n-1}2(h_i+h_{i+1})\left\|e^{''}\right\|^2_{L^2(0,1)}\\ &\le 8\delta^2\left(2+\left\|y^{''}\right\|^2_{L^2(0,1)}\right)\left\|e^{''}\right\|^2_{L^2(0,1)}\\ &\le 8\delta^2\left(\sqrt{2}+\left\|y^{''}\right\|_{L^2(0,1)}\right)^2\left(1+2\left\|y^{''}\right\|_{L^2(0,1)}\right)^2\end{aligned}$$

By the estimations for I_1 and I_2, we can obtain

$$\begin{aligned}&\left(\left\|e^{'}\right\|_{L^2(0,1)}-h\left(\left\|y^{''}\right\|_{L^2(0,1)}+\frac{1}{2}\right)\right)^2\\ &\le\left(h\left\|y^{''}\right\|_{L^2(0,1)}+\frac{h}{2}+2\sqrt{\delta}\left(1+2\left\|y^{''}\right\|_{L^2(0,1)}\right)\right)^2.\end{aligned}$$

Therefore, we have

$$\begin{aligned}\left\|e^{'}\right\|_{L^2(0,1)} &\le 2h\left\|y^{''}\right\|_{L^2(0,1)}+h+2\sqrt{\delta}+4\sqrt{\delta}\left\|y^{''}\right\|_{L^2(0,1)}\\ &= \left(2h+4\sqrt{\delta}\right)\left\|y^{''}\right\|_{L^2(0,1)}+h+2\sqrt{\delta}. \qquad (3.10)\end{aligned}$$

By using the triangle inequality, finally we obtain

$$\begin{aligned}\left\|f_*^{'}-y^{'}\right\|_{L^2(0,1)} &\le \left\|e^{'}\right\|_{L^2(0,1)}+\left\|s^{'}-y^{'}\right\|_{L^2(0,1)}\\ &\le \left(2h+4\sqrt{\delta}\right)\left\|y^{''}\right\|_{L^2(0,1)}+h+2\sqrt{\delta}+\frac{h}{\pi}\left\|y^{''}\right\|_{L^2(0,1)}. \qquad (3.11)\end{aligned}$$

This completes the proof.

3.4. **Proof of Theorem 2.5:** We will divide the proof into 4 steps.

Step 1: Assume that the conclusion of the Theorem is not correct. This means that there exist two sequences δ^m, Δ^m, $m = 1, 2, \cdots$, and a constant $C > 0$ such that

$$\delta^m \to 0, \quad h^m \to 0, \qquad as \quad m \to \infty$$

and

$$\left\| f_*^{''}(x; \delta^m, h^m) \right\|_{L^2(0,1)} \le C.$$

Here h^m is the maximum mesh size of the grid Δ^m, i.e. $h^m = \max_{0\le i\le n-1} h_i^m$. We use the notation $f_*^{''}(x; \delta^m, h^m)$ to indicate that $f_*(x)$ depends on δ^m and h^m.

From the theory of Sobolev spaces, we know that there exists a function $g \in H^2(0,1)$ which satisfies

$$\left\| g^{''} \right\|_{L^2(0,1)} \le C \tag{3.12}$$

and

$$\lim_{m\to 0} \| f_*(\delta^m, h^m, x) - g(x) \|_{C[0,1]} = 0. \tag{3.13}$$

Step 2: Let $\phi(g) = \|g - y\|_{C[0,1]}$ and $Y = \{g \in H^2(0,1) \,|\, g(0) = y(0),\, g(1) = y(1)\}$.

For sufficient small $\delta > 0$, we want to find function $\widetilde{f}_\delta$ such that

(1) $\widetilde{f}_\delta(0) = y(0), \quad \widetilde{f}_\delta(1) = y(1)$;
(2) $\left\| \widetilde{f}_\delta^{''} \right\|_{L^2(0,1)} \le \frac{1}{\sqrt{\delta}}$;
(3) $\phi(\widetilde{f}_\delta) \le \inf_{g\in H_\delta} \phi(g) + \delta$. Here $H_\delta = \left\{ g \in Y \mid \left\| g^{''} \right\|_{L^2(0,1)} \le \frac{1}{\sqrt{\delta}} \right\}$.

By the definition, the existence of $\widetilde{f}_\delta$ is obvious.

Now we want to prove

$$\phi(\widetilde{f}_\delta) \to 0. \tag{3.14}$$

We assume the conclusion (3.14) is not true. Then there exist a constant $C_1 > 0$ and a sequence δ_k, $k = 1, 2 \cdots$, such that

$$\delta_k \to 0, \qquad as \quad k \to \infty$$

and

$$\phi(\widetilde{f}_{\delta_k}) \ge C_1.$$

Since Y is dense in $C[0,1]$, for the function $y \in C[0,1] \setminus H^2(0,1)$, there exists a function $z \in Y$ such that

$$\phi(z) = \|z - y\|_{C[0,1]} < \frac{C_1}{2}.$$

We denote $B = \left\|z''\right\|_{L^2(0,1)}$.

Since $\delta_k \to 0$ as $k \to 0$, there exists a constant $K > 0$ such that

$$B < \frac{1}{\sqrt{\delta_k}}, \quad \delta_k < \frac{C_1}{2}, \qquad for \quad k \geq K.$$

Therefore it holds that

$$\left\|z''\right\|_{L^2(0,1)} < \frac{1}{\sqrt{\delta_K}}.$$

By the definition of $\widetilde{f}_\delta$, we obtain

$$\phi(\widetilde{f}_{\delta_k}) \leq \phi(z) + \delta_k < \frac{C_1}{2} + \frac{C_1}{2} = C_1.$$

This is a contradiction.

The conclusion (3.14) is correct.

Step 3: In this step, we will prove

$$\lim_{\delta \to 0} \Phi(f_*) = 0.$$

Firstly, we have

$$\begin{aligned}
\Phi(\widetilde{f}_\delta) &= \sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2} (\widetilde{y}_i - \widetilde{f}_\delta(x_i))^2 + \delta^2 \left\|\widetilde{f}_\delta''\right\|^2_{L^2(0,1)} \\
&\leq 2\delta^2 + 2\sum_{i=1}^{n-1} \frac{h_i + h_{i+1}}{2} (y - \widetilde{f}_\delta(x_i))^2 + \delta \\
&\leq \delta + 2\delta^2 + 2\phi(\widetilde{f}_\delta)
\end{aligned}$$

Since $\lim_{\delta \to 0} \phi(\widetilde{f}_\delta) = 0$, we get

$$\lim_{\delta \to 0} \Phi(\widetilde{f}_\delta) = 0.$$

Therefore we have

$$\lim_{\delta \to 0} \Phi(f_*) = 0. \tag{3.15}$$

Step 4: Let $\varepsilon > 0$ be an arbitrary small number.

By the definition of the integral, we have

$$\lim_{h^m\to 0}\sum_{i=1}^{n^m-1}\frac{h_i^m+h_{i+1}^m}{2}(g(x_i^m)-y(x_i^m))^2=\|g-y\|^2_{L^2(0,1)}.$$

Therefore, there exists a $M>0$ such that, for any $m>M$, it holds that

$$\|g-y\|^2_{L^2(0,1)}\le\sum_{i=1}^{n^m-1}\frac{h_i^m+h_{i+1}^m}{2}(g(x_i^m)-y(x_i^m))^2+\varepsilon \tag{3.16}$$

By (3.12) and (3.13), we have that there exists a constant $M_1>0$ such that, for $m>M_1$, it holds that

$$\|f_*(\delta^m,h^m,x)-g(x)\|^2_{C[0,1]}<\varepsilon \tag{3.17}$$

and

$$(\delta^m)^2<\frac{\varepsilon}{C} \tag{3.18}$$

By (3.15), we know that there exists a constant $M_2>0$ such that, for $m>M_2$, it holds that

$$|\Phi(f_*)|<\varepsilon. \tag{3.19}$$

Therefore, by (3.16) – (3.19), we know that, $m>\max(M,M_1,M_2)$, it holds that

$$\begin{aligned}\|g-y\|^2_{L^2(0,1)} &\le 3\sum_{i=1}^{n^m-1}\frac{h_i^m+h_{i+1}^m}{2}\Big(g(x_i^m)-f_*(x_i^m;\delta^m,h^mn)\Big)^2\\ &\quad+3\sum_{i=1}^{n^m-1}\frac{h_i^m+h_{i+1}^m}{2}\Big(f_*(\delta^m,h^m,x_i^m)-\widetilde{y}(x_i^m)\Big)^2\\ &\quad+3\sum_{i=1}^{n^m-1}\frac{h_i^m+h_{i+1}^m}{2}\Big(\widetilde{y}(x_i^m)-y(x_i^m)\Big)^2+\varepsilon\\ &\le 3\varepsilon+3\Phi(f_*(\delta^m,h^m,x))+3(\delta^m)^2C+\varepsilon\\ &\le 10\varepsilon\end{aligned}$$

Since ε is an arbitrary positive number, we obtain

$$g=y.$$

From the Step 1, we know that $g\in H^2(0,1)$. This contradicts with the assumption that $y\notin H^2(0,1)$.

This completes the proof.

4. Numerical examples and applications

For testing our algorithm. we calculate the examples in the section on a SGI 540 NT Workstation computer with 2 CPUs and 256M memory. The programming language is MATLAB.

4.1. **Example 1: Numerical Differentiation of A Smooth function.**

We first consider an example that the exact solution y is a smooth function. Our method is compared with the method in [10] [16].

We take $y = 2x^3 + 3x^2 + 4x + 5$. The parameters are chosen as $n = 200$, $\delta = 0.0001$. 200 random points are distributed in (-1,1). Figure 1 is based on the method of [10][16], while Figure 2 is based on the method of this paper. In both of Figure 1 and Figure 2, the dotted line represents y' and solid line is f'_*.

We find that y' and f'_* almost match, that means the both of the methods are applicable and these two method have the same precision. But the computational times are different. The method of [10][16] needs 15 seconds and our method only needs 0.61 seconds.

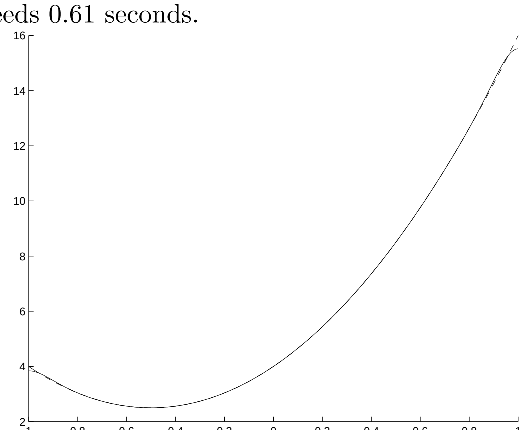


Figure 1 Pictures of y' and f'_* of [10][16]

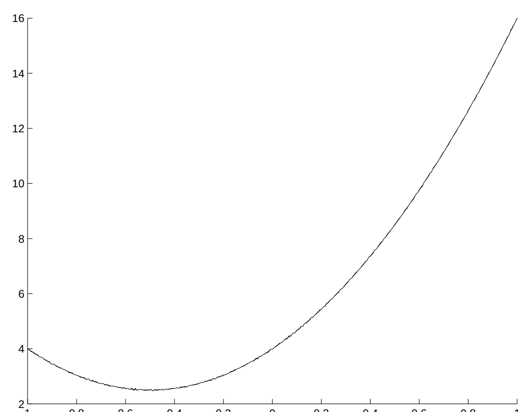


Figure 2 Pictures of y' and f'_*

We change the parameters of n and δ and compare the results again. We choose $n = 400$ and $\delta = 0.0001$. The results show that the precision is still similar, but one needs 133.6 seconds and the other only need 4 seconds.

4.2. **Example 2: Numerical Differentiation of A Discontinuous Function.**

We consider the case that y is a discontinuous function. Since the values of the function are only given at finite points, we still can do the process which we do for the smooth function. According to Theorem 2.5, we know that the norm of $f_*^{''}$ will blow up as $\delta \to 0$, $h \to 0$. We can see it clearly from Figure 5 below.

Let

$$y = \begin{cases} 3x^3 + 4x^2 + 5, x \in (-1, 0) \\ 4x^3 + 6x, x \in [0, 1) \end{cases} \tag{4.1}$$

See Figure 3. We know that 0 is the discontinuous point of this function.

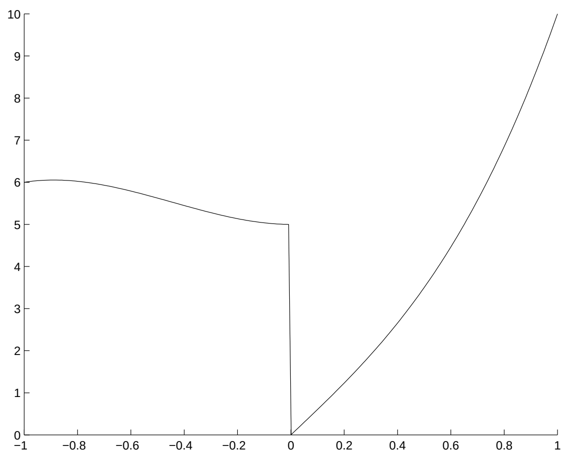


Figure 3 Picture of y

It is the same as previous example that the parameters are chosen as $n = 200$, $\delta = 0.0001$. 200 random points are distributed in (-1,1).

The $y^{'}(t)$ (except $t = 0$) is shown in Figure 4 and the $f_*^{'}$ we calculated by our method is shown in Figure 5.

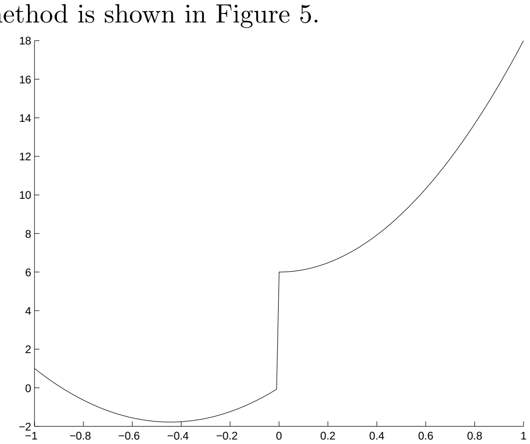


Figure 4 Picture of $y^{'}$

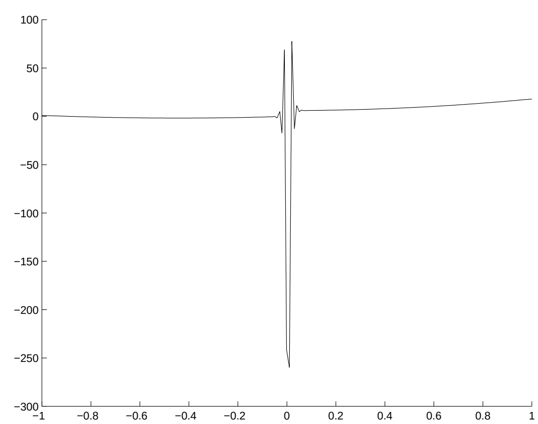


Figure 5 Picture of $f_*^{'}$

Remark 4.1. Since the some values of $f_*^{'}$ are very large near 0, we use different scale coordinates for these two figures. This is why these two figures look different. Actually the values of $f_*^{'}(t)$ and $y^{'}(t)$ are very close for t a little far from 0.

We can calculate $f_*^{''}$ on the whole interval and some small subinterval. We can have some detail information about the discontinuous points of y.
(1). First we calculate the norm of $f_*^{''}$ on the whole interval. We have $\left\| f_*^{''} \right\|_{L^2(-1,1)} = 32692$. It is very large. According to the result in this paper, we know that there may exist discontinuous points of y in (-1,1).
(2). We calculate the norm of $f_*^{''}$ on the subinterval. We have $\left\| f_*^{''} \right\|_{L^2(-1,-0.1)} = 413.6$, $\left\| f_*^{''} \right\|_{L^2(-0.1,0.1)} = 32686$ and $\left\| f_*^{''} \right\|_{L^2(0.1,1)} = 479.5$. Then we know that the discontinuous points may be in the interval (-0.1,0.1).
(3). We repeat the second step. Then we can find a small interval which may contain the discontinuous point.

4.3. **One Application.** Numerical differentiation is an important problem. We will show that the method we proposed in this paper may be applied to some important practical problems. Here we just give a very simple, but interesting application in CT (Computerized Tomography) ([13]).

Assume that an object whose attenuation coefficient with respect to X-rays at the point x is $f(x)$. We scan the cross-section by a thin X-ray beam L of unit intensity. The intensity past the object is

$$e^{-\int_L f(x)dx}.$$

We denote

$$g(L) = \int_L f(x)dx.$$

The main problem in CT is to recover the function f from g.

Next we will show that, by our numerical differentiation method, we can find the discontinuous points of $f(x)$. These discontinuous points represent the interface of different materials. Then the shape of the object can be reconstructed.

We consider the simplest case that the object's cross-section is an equilateral triangle which we denote as D. The attenuation coefficient is 0 outside the object and 1 inside the object, i.e.

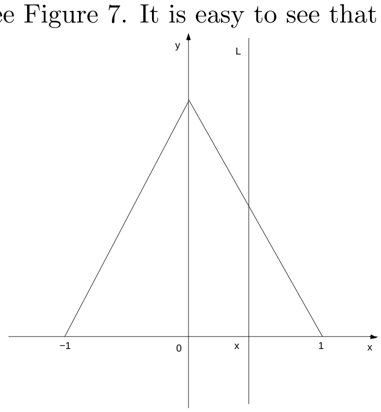
$$f(x) = \begin{cases} 1, x \in D \\ 0, x \notin D \end{cases} \tag{4.2}$$

See Figure 6.

$g(x)$ can be calculated directly

$$g(x) = \begin{cases} \sqrt{3}(1-x), 0 \leq x < 1 \\ \sqrt{3}(1+x), -1 \leq x < 0 \\ 0, else \end{cases} \tag{4.3}$$

See Figure 7. It is easy to see that there are 3 discontinuous points.



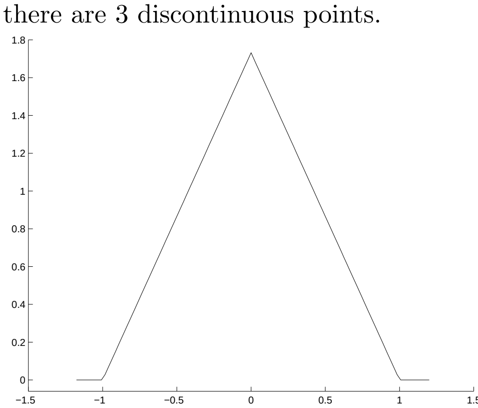


Figure 6 Picture of D and L

Figure 7 Picture of g

By our method, we choose 200 random points as x_i, $i = 0, 1, 2, \cdots, 200$, and reconstruct $g^{'}(x)$ from $g(x_i) + \epsilon_i$ (Here ϵ_i is a random errors whose value is less than 0.001.) The second order derivative $f_*^{''}$ is shown in Figure 8.

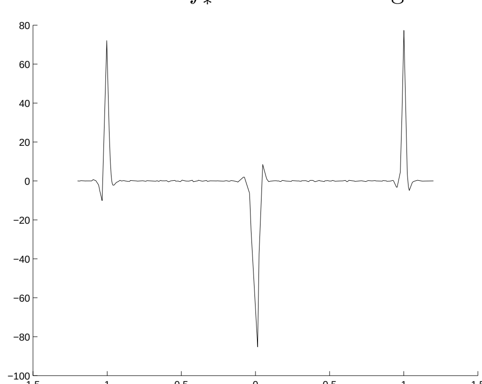


Figure 8 Picture of $f_*^{''}$

From Figure 8, we can find that, the values of f'_* are quite large near 3 points: $-1, 0, 1$, and are almost 0 at other points. Moreover, we can calculate the norm of f'_* on some intervals. By the similar way used for the Example 2, we can easily find the discontinuous points.

Remark 4.2. Here we only consider the integral along one direction. We also can do the same process along the other directions. The same results can be obtained. It seems that, from the information along the three directions, we can reconstruct one convex polygon. This research is in progress.

5. Conclusions

Numerical differentiation problem arises in many branches of sciences and engineering. In this paper, we proposed a method which is based on the Tikhonov regularization and the conditional stability estimation. It has been shown that our method is an easily realizing method and can be used to determine the discontinuous points of the exact solution.

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