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STABLE NUMERICAL DIFFERENTIATION: WHEN IS IT POSSIBLE?

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ABSTRACT. Two principally different statements of the problem of stable numerical differentiation are considered. It is analyzed when it is possible **in principle** to get a stable approximation to the derivative f' given noisy data f_δ. Computational aspects of the problem are discussed and illustrated by examples. These examples show the practical value of the new understanding of the problem of stable differentiation.

1. INTRODUCTION

In many applications one has to estimate a derivative f' given the noisy values of the function f to be differentiated. As an example we refer to the analysis of photoelectric response data (see [11]). The goal of that experiment is to determine the relationship between the intensity of light falling on certain plant cells and their rate of uptake of various substances. Rather than measuring the uptake rate directly, the experimentalists measure the amount of each substance not absorbed as a function of time, the uptake rate being defined as minus the derivative of this function. As for the other example, one can mention the problem of finding the heat capacity c_p of a gas as a function of temperature T. Experimentally one measures the heat content $q(T) = \int_{T_0}^{T} c_p(\tau)d\tau$, and the heat capacity is determined by numerical differentiation.

One can give many other examples of practical problems in which one has to differentiate noisy data. In navigation problems one selects the direction of the motion of a ship by the maximum of a certain univalent curve, called the navigation characteristic. This direction can be obtained by differentiation of this curve. Since the navigation characteristic is communicated with some errors, one has to differentiate it numerically in order to find its maximum. In [18], p. 94, the shape of a convex obstacle is found by differentiation of a support function of this obstacle. The support function is found from the experimentally measured scattering data, and by this reason the support function is noisy. In [19], pp.81-92, optimal estimates for the derivatives of random functions

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are obtained. In [22], p. 438, numerical differentiation of functions, contaminated by random noise is discussed. The noise has zero mean value and finite variance, and is identically distributed independently of the point x. It is proved that in this case the error of an optimal formula of numerical differentiation can be made $O(p^{-0.25}\epsilon)$, where p is the number of observation points and ϵ is the error for a noise which is non-random (see the precise formulation of the result in [22]).

The differentiation of noisy data is an ill-posed problem: small (in some norm) perturbations of a function may lead to large errors in its derivative. Indeed, if one takes $f_\delta = f + \delta \sin\left(\frac{t}{\delta^2}\right)$, $f' \in L^\infty(0,1)$, then $||f_\delta - f||_\infty = \delta$ and $||f'_\delta - f'||_\infty = \frac{1}{\delta}$, so that small in $L^\infty(0,1)$-norm perturbations of f result in large perturbations of f' in $L^\infty(0,1)$-norm.

Various methods have been developed for stable numerical differentiation of f given f_δ, $||f_\delta - f|| \le \delta$. We mention three groups of methods:

1) regularized difference methods with a step size $h = h(\delta)$ being a regularization parameter, see [13], where this idea was proposed for the first time, and [16], [19], [20]. As an example of such a method one may consider:

$$R_{h(\delta)} f_\delta(x) := \begin{cases} \frac{1}{h}(f_\delta(x+h) - f_\delta(x)), & 0 < x < h, \\ \frac{1}{2h}(f_\delta(x+h) - f_\delta(x-h)), & h \le x \le 1-h, \\ \frac{1}{h}(f_\delta(x) - f_\delta(x-h)), & 1-h < x < 1, \quad h > 0. \end{cases} \tag{1.1}$$

If $f_\delta \in L^\infty(0,1)$, and $f \in W^{2,p}(0,1)$, where $W^{n,p}(0,1)$ is the Sobolev space of functions whose n-th derivative belongs to $L^p(0,1)$, $||f_\delta - f||_p \le \delta$, then

$$||R_{h(\delta)} f_\delta - f'||_p \le ||R_{h(\delta)}(f_\delta - f)||_p + ||R_{h(\delta)} f - f'||_p$$

$$\le \frac{2\delta}{h} + \frac{N_{2,p} h}{2}, \tag{1.2}$$

where $N_{2,p}$ is an estimation constant: $||f''||_p \le N_{2,p}$. The error in the interval $h \le x \le 1-h$ can be estimated slightly better (by a quantity $\frac{\delta}{h} + \frac{N_{2,p}h}{2}$). In this paper by $||\cdot||_p$ we denote $||\cdot||_{L^p(0,1)}$. The right-hand side of (1.2) attains the absolute minimum $2\sqrt{\delta N_{2,p}}$ at $h = h_{2,p}(\delta) := 2\left(\frac{\delta}{N_{2,p}}\right)^{\frac{1}{2}}$, while if one uses the error estimate for the interval $h \le x \le 1-h$, then one gets the absolute minimum $\sqrt{2\delta N_{2,p}}$ at $h = \left(\frac{2\delta}{N_{2,p}}\right)^{\frac{1}{2}}$. When the function $f \in W^{3,p}(0,1)$, one can modify (1.1) near the ends so that it has the order $O(h^2)$ of the error of approximation as $h \to 0$, and results in an algorithm of order $\delta^{2/3}$. For example one can take

$$R_{h(\delta)} f_\delta(x) := \begin{cases} \frac{1}{2h}(4f_\delta(x+h) - f_\delta(x+2h) - 3f_\delta(x)), & 0 < x < 2h, \\ \frac{1}{2h}(f_\delta(x+h) - f_\delta(x-h)), & 2h < x < 1-2h, \\ \frac{1}{2h}(3f_\delta(x) + f_\delta(x-2h) - 4f_\delta(x-h)), & 1-2h < x < 1. \end{cases} \tag{1.3}$$

The difference methods use only local values of the function f_δ, which is natural when one estimates a derivative, and these methods are very simple, which is an advantage.

2) An alternative approach is first to smooth f_δ by a mollification with a certain kernel, for example with a Gaussian kernel, or to use a mollification by splines, and then to differentiate the resulting smooth approximation, see ([27], [10], [7]). If one applies mollification with the Gaussian kernel $w_h(x) := \frac{1}{h\sqrt{\pi}} \exp\left(-\frac{x^2}{h^2}\right)$, $x \in \mathbb{R}$, $h > 0$, then $(M_{h(\delta)})' : L^2(0,1) \to L^2(0,1)$,

$$(M_{h(\delta)})' f_\delta(x) := (w_h' \star f_\delta)(x) := \int_0^1 w_h'(x-s) f_\delta(s) ds, \tag{1.4}$$

where $*$ stands for the convolution, $f_\delta \in L^2(0,1)$, and $||f_\delta - f||_2 \leq \delta$. Assume that $f \in H^1(0,1)$ with $f(0) = f(1) = 0$ and $||f''||_2 \leq N_{2,2}$. One has

$$||(M_{h(\delta)})' f_\delta - f'||_2 \leq ||(M_{h(\delta)})'(f_\delta - f)||_2 + ||(M_{h(\delta)})' f - f'||_2 \tag{1.5}$$

From the Cauchy inequality the first term in the right-hand side of (1.5) can be estimated as follows:

$$||(M_{h(\delta)})'(f_\delta - f)||_{L^2(0,1)} = ||w_h' \star (f_\delta - f)||_{L^2(0,1)} \leq ||w_h' \star (f_\delta - f)||_{L^2(\mathbb{R})}$$

$$\leq ||w_h'||_{L^1(\mathbb{R})} ||f_\delta - f||_{L^2(0,1)} \leq \frac{2\delta}{h\sqrt{\pi}}, \tag{1.6}$$

because $||w_h'||_{L^1(\mathbb{R})} = -2 \int\limits_0^\infty w_h'(s) ds = 2w_h(0) = \frac{2}{h\sqrt{\pi}}$. By a partial integration one gets:

$$(w_h' \star f)(x) = \int\limits_0^1 w_h'(x-s) f(s) ds = \int\limits_0^1 w_h(x-s) f'(s) ds = (w_h \star f')(x). \tag{1.7}$$

To complete the argument one uses the inequality

$$||w_h \star z - z||_{L^2(\mathbb{R})} \leq h||z'||_{L^2(0,1)} \tag{1.8}$$

for every $z \in H^1(0,1)$ with $z(0) = z(1) = 0$. Here the above functions z are extended from $[0,1]$ to $\mathbb{R}$ by zero.

To verify (1.8) define the Fourier transform by

$$(\mathcal{F}z)(t) := \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} z(s) e^{ist} ds, \quad t \in \mathbb{R}.$$

Using Parseval's equation, one gets:

$$||w_h \star z - z||_{L^2(\mathbb{R})} = ||\mathcal{F}(w_h \star z - z)||_{L^2(\mathbb{R})} = ||(\sqrt{2\pi}\mathcal{F}w_h - 1)\mathcal{F}z||_{L^2(\mathbb{R})}$$

$$= \left\| \frac{1}{-it}(\sqrt{2\pi}\mathcal{F}w_h - 1)\mathcal{F}z' \right\|_{L^2(\mathbb{R})} \leq \left\| \frac{1}{-it}(\sqrt{2\pi}\mathcal{F}w_h - 1) \right\|_{L^\infty(\mathbb{R})} ||z'||_{L^2(0,1)}. \tag{1.9}$$

Since

$$\varphi_h(t) := \frac{1}{it}(1 - \sqrt{2\pi}\mathcal{F}w_h) = \frac{1}{it}\left[1 - e^{-h^2t^2/4}\right], \quad t \in \mathbb{R},$$

and $\frac{1-e^{-\tau^2}}{\tau} \leq 2$, for all $\tau > 0$, estimate (1.9) yields inequality (1.8). Thus from (1.7) and (1.8) one obtains

$$||(M_{h(\delta)})'f - f'||_2 \leq ||w_h \star f' - f'||_2 \leq hN_{2,2}. \tag{1.10}$$

Finally, combining (1.5), (1.6) and (1.10) one gets

$$||(M_{h(\delta)})'f_\delta - f'||_2 \leq \frac{2\delta}{h\sqrt{\pi}} + hN_{2,2} := \varepsilon_2.$$

The choice $h = h_{2,2}(\delta) = \sqrt{\frac{2\delta}{N_{2,2}\sqrt{\pi}}}$ leads to the estimate $\varepsilon_2 \leq 2\sqrt{2/\sqrt{\pi}}\sqrt{\delta N_{2,2}}$.

3) The third group of methods uses variational regularization for solving ill-posed problems ([12], [26]). One applies variational regularization to a Volterra integral equation

$$Au(x) := \int_0^x u(s)ds = f(x). \tag{1.11}$$

For example, if the noisy data f_δ are given, $||f_\delta - f||_2 \leq \delta$, then one minimizes the functional

$$F_0(u) := ||Au - f_\delta||_2^2 + \alpha||u||_2^2$$

or

$$F_m(u) := ||Au - f_\delta||_2^2 + \alpha||u^{(m)}||_2^2, \quad m > 0,$$

where $\alpha >$ is a regularization parameter. One proves that for a suitable choice of α, $\alpha = \alpha(\delta)$, the above functionals have a unique minimizer u_δ and $||u_\delta - f'||_2 \to 0$ as $\delta \to 0$. An optimal choice of the regularization parameter α in this approach is a nontrivial problem. Some methods for choosing $\alpha = \alpha(\delta)$ are presented in [9], [4].

The above methods have been discussed in the literature (see, for example, [5], [6], [1], [2], [8]), and their analysis is not our goal. Our goal is to study two principally different statements of the problem of stable numerical differentiation, and to understand when it is possible in principle to get a stable approximation to f' given noisy data f_δ. In [25] a new notion of regularizer is introduced. Our treatment of the stable differentiation is an example of application of this new notion. In [24] a regularization method for unbounded linear and nonlinear operators is discussed.

2. Statements of the problem of stable numerical differentiation

First, we recall some standard definitions. The problem of finding a solution u to the equation

$$A(u) = f, \quad A : X \to Y, \tag{2.1}$$

where X and Y are Banach spaces, A is an operator, possibly nonlinear, is *well-posed* (in the sense of J.Hadamard) if the following conditions hold:

a) for every element $f \in Y$ there exists a solution $u \in X$;

b) this solution is unique;

c) the problem is stable under small perturbations of the initial data in the sense:

$$||u_\delta - u||_X \to 0 \quad \text{if} \quad ||f_\delta - f||_Y \to 0, \quad \text{where} \quad A(u_\delta) := f_\delta.$$

If at least one of the conditions a), b) or c) is violated, then the problem is called *ill-posed.* The problem of numerical differentiation can be written as

$$A(u) := \int_0^x u(s)ds = f, \quad A : X = L^p(0,1) \to L^p(0,1), \quad f(0) = 0. \tag{2.2}$$

We study the cases $p = 2$ and $p = \infty$ in detail. Problem (2.2) is solvable only if $f' \in X$. So, condition a) is not satisfied, condition c) is not satisfied either, and condition b) is satisfied. Therefore, problem (2.2) is ill-posed.

Practically, one does not know f and the only information available for computational processing is f_δ together with an *a priori* information about f, for example, one may know that $f \in \mathcal{K}^p_{\delta,a}$, where

$$\mathcal{K}^p_{\delta,a} := \{f : f \in W^{a,p}(0,1),\ ||f^{(a)}||_p \le N_{a,p} < \infty,\ ||f_\delta - f||_p \le \delta\}, \tag{2.3}$$

$a = 0$,$a = 1$, or $1 < a \le 2$. For $1 < a < 2$

$$||f^{(a)}||_p := \sup_{x,y\in(0,1),\, x\ne y} \frac{||f'(x) - f'(y)||_p}{|x-y|^{a_0}}, \quad a = 1 + a_0, \quad 0 < a_0 < 1. \tag{2.4}$$

Therefore given $\delta > 0$ and f_δ one has to estimate f' for *any* $f \in \mathcal{K}^p_{\delta,a}$ and the problem of stable numerical differentiation has to be understood in the following sense:

Problem I:
Find a linear or nonlinear operator $R_{h(\delta)}$ such that

$$\sup_{f\in\mathcal{K}^p_{\delta,a}} ||R_{h(\delta)} f_\delta - f'||_p \le \eta(\delta) \to 0 \quad \text{as} \quad \delta \to 0, \tag{2.5}$$

where $\eta(\delta)$ is some positive continuous function of $\delta \in (0, \delta_0)$, and $\delta_0 > 0$ is some number.

The traditional formulation of the problem of stable numerical differentiation is different from the above:

Problem II:
Find a linear or nonlinear operator $R_{h(\delta)}$ such that

$$\sup_{f_\delta \in \mathcal{B}^p_{\delta,f}} ||R_{h(\delta)} f_\delta - f'||_p \leq \eta(\delta, f) \to 0 \quad as \quad \delta \to 0, \tag{2.6}$$

where $\mathcal{B}^p_{\delta,f} := \{f_\delta : ||f_\delta - f||_p \leq \delta\}$ *and* $f \in \mathcal{K}^p_{\delta,a}$ *is* **fixed**,

or even in a weaker form:

Find $R_{h(\delta)}$ *such that*

$$||R_{h(\delta)} f_\delta - f'||_p \leq \eta(\delta, f) \to 0 \quad as \quad \delta \to 0 \tag{2.7}$$

for a **fixed** $f \in \mathcal{K}^p_{\delta,a}$ *and* **fixed** *family* $f_\delta \in \mathcal{B}^p_{\delta,f}$.

Note the **principal difference** in the statements of Problems I and II of stable numerical differentiation: in Problem I the data are $\{f_\delta, N_{a,p}\}$, f is arbitrary in the set $\mathcal{K}^p_{\delta,a}$, and we wish to find a stable approximation of f', which is valid uniformly with respect to $f \in \mathcal{K}^p_{\delta,a}$. On the other hand, in Problem II it is assumed that $f \in \mathcal{K}^p_{\delta,a}$ is fixed and the approximation of f' is either uniform with respect to $f_\delta \in \mathcal{B}^p_{\delta,f}$ or holds for a particular family $f_\delta \in \mathcal{B}^p_{\delta,f}$. Since in practice we do not know f and we do know just one family f_δ, Problem I is much more important practically than Problem II. In this paper we show when one can obtain, in principle, a stable approximation of f' in the sense formulated in Problems I and II, and when it is not possible, in principle, to obtain such an approximation of f' from noisy data.

The main result on the stable numerical differentiation problem in the first formulation is stated in Theorem 2.1:

Theorem 2.1. *There does not exist an operator* $R_{h(\delta)} : L^p(0,1) \to L^p(0,1)$, *linear or nonlinear, for* $p = 2$ *and* $p = \infty$, *such that inequality (2.5) holds for* $a \leq 1$. *If* $a \leq 1$, *then*

$$\gamma^{\infty}_{\delta,a} := \inf_{R_{h(\delta)}: L^p(0,1) \to L^p(0,1)} \sup_{f \in \mathcal{K}^p_{\delta,a}} ||R_{h(\delta)} f_\delta - f'||_p \geq c > 0, \quad p = 2, \infty. \tag{2.8}$$

If $a > 1$ *and* $p \geq 1$, *then there does exist an operator* $R_{h(\delta)}$ *such that (2.5) holds. For example, one can use* $R_{h(\delta)}$ *defined in (1.1) with*

$$h = h_a(\delta) := \begin{cases} \left(\frac{2\delta}{a_0 N_{a,p}}\right)^{\frac{1}{a}}, & a = 1 + a_0, \quad 0 < a_0 < 1, \\ 2\left(\frac{\delta}{N_{2,p}}\right)^{\frac{1}{2}}, & a = 2. \end{cases} \tag{2.9}$$

The error of the corresponding differentiation formula is

$$\eta(\delta) := \begin{cases} a(N_{a,p})^{\frac{1}{a}} \left(\frac{2\delta}{a_0}\right)^{\frac{a_0}{a}}, & a = 1 + a_0, \quad 0 < a_0 < 1, \\ 2(\delta N_{2,p})^{\frac{1}{2}}, & a = 2. \end{cases} \tag{2.10}$$

The main result on the stable numerical differentiation problem in the second formulation is stated in Theorem 2.2:

Theorem 2.2. *If $a = 1$, then there exists an operator $R_{h(\delta)} : L^2(0,1) \to L^2(0,1)$, such that inequality (2.6) holds.*

The principal difference is: for $a = 1$ one cannot differentiate stably in the sense formulated in Problem I. In the sense of Problem II stable differentiation is possible in principle. However the approximation error, $||R_{h(\delta)}f - f'||_2$, cannot be estimated, and this error $\eta(\delta, f)$ may go to zero arbitrarily slowly as $\delta \to 0$. This is in sharp contrast with the practically computable error estimate given in (2.10). Moreover, no matter how small the error bound $\delta > 0$ is, there exists a function $f \in \mathcal{K}^2_{\delta,1}$, such that not only $R_{h(\delta)}$ (with any fixed function $h(\delta)$), defined in (3.14), but *any other operator* $R_{h(\delta)}$, linear or nonlinear, will satisfy the inequality $||R_{h(\delta)}f - f'||_2 \geq c > 0$, where $c > 0$ does not depend on δ. This follows from (2.8).

3. Proofs

Proof of Theorem 2.1

First, consider the case $p = \infty$. Take

$$f_1(x) := -\frac{M}{2}x(x-2h), \quad 0 \leq x \leq 2h. \tag{3.1}$$

Extend $f_1(x)$ from $(0, 2h)$ to $(2h, 1)$ by zero and denote the extended function by $f_1(x)$ again. Then $f_1(x) \in W^{1,\infty}(0,1)$ and the norms $||f^{(a)}||_\infty$, $a = 0$ and $a = 1$ are preserved. Define $f_2(x) = -f_1(x)$, $x \in (0,1)$. Note that

$$\sup_{x\in(0,1)} |f_k(x)| = \frac{Mh^2}{2}, \quad k = 1,2. \tag{3.2}$$

Choose $h = h_\infty := h_\infty(\delta) := \sqrt{\frac{2\delta}{M}}$, so that

$$\frac{Mh_\infty^2}{2} = \delta, \tag{3.3}$$

Then for $f_\delta(x) \equiv 0$ one has: $||f_k - f_\delta||_\infty = \delta$, $k = 1,2$. Let $(R_{h(\delta)}f_\delta)(0) = (R_{h(\delta)}0)(0) := b$. One gets

$$\begin{aligned}\gamma^\infty_{\delta,a} &:= \inf_{R_{h(\delta)}} \sup_{f\in\mathcal{K}^\infty_{\delta,a}} ||R_{h(\delta)}f_\delta - f'||_\infty \geq \inf_{R_{h(\delta)}} \max_{k=1,2} ||R_{h(\delta)}f_\delta - f'_k||_\infty \\ &\geq \inf_{R_{h(\delta)}} \max_{k=1,2} ||R_{h(\delta)}f_\delta(0) - f'_k(0)||_\infty \\ &= \inf_{b\in\mathbb{R}} \max\{|b - Mh_\infty|, |b + Mh_\infty|\} = Mh_\infty. \end{aligned} \tag{3.4}$$

If $h_\infty = \sqrt{\frac{2\delta}{M}}$, then $Mh_\infty = \sqrt{2\delta M}$. If $a = 0$, then (3.2) implies that $f_k \in \mathcal{K}^\infty_{\delta,0}$, $k = 1, 2$, with $N_{0,\infty} := \frac{Mh^2_\infty}{2} = \delta$. For any fixed $\delta > 0$ and $N_{0,\infty} = \delta$ the constant M in (3.1) can be chosen arbitrary. Therefore inequality (3.4) proves that (2.5) is false in the class $\mathcal{K}^\infty_{\delta,0}$ and, in fact, $\gamma^\infty_{\delta,0} \to \infty$ as $M \to \infty$.

Suppose now that $f \in \mathcal{K}^\infty_{\delta,1}$. One has

$$||f_1'||_\infty = ||f_2'||_\infty = \sup_{0\le x\le 2h_\infty} |M(x - h_\infty)| = Mh_\infty. \tag{3.5}$$

Thus, for given δ and $N_{1,\infty}$ one can take $h = h_\infty := \sqrt{\frac{2\delta}{M}}$, so that $||f_k - f_\delta||_\infty = \delta$, $k = 1, 2$, holds, and then take M so that $N_{1,\infty} = \sqrt{2\delta M}$. For these h_∞ and M the functions $f_k \in \mathcal{K}^\infty_{\delta,1}$, $k = 1, 2$. One obtains from (3.4) the following inequality

$$\gamma^\infty_{\delta,1} \ge N_{1,\infty} > 0 \quad \text{as} \quad \delta \to 0, \tag{3.6}$$

which implies that estimate (2.5) is false in the class $\mathcal{K}^\infty_{\delta,1}$.

Now let $p = 2$. For f_1 defined in (3.1) one has

$$||f_1||_{L^2(0,2h)} = \frac{2}{\sqrt{15}} Mh^{\frac{5}{2}}, \quad ||f_1'||_{L^2(0,2h)} = \sqrt{\frac{2}{3}} Mh^{\frac{3}{2}}. \tag{3.7}$$

Extend $f_1(x)$ from $(0, 2h)$ to $(2h, 1)$ by zero and denote the extended function $f_1(x)$ again. Then $f_1 \in W^{1,2}(0, 1)$, $||f_1||_{L^2(0,1)} = c_1 Mh^{\frac{5}{2}}$, and $||f_1'||_{L^2(0,1)} = c_2 Mh^{\frac{3}{2}}$. Define $f_2(x) = -f_1(x)$, $f_\delta(x) \equiv 0$, $x \in (0, 1)$.

Choose $h = h_2 := \left(\frac{\delta}{c_1 M}\right)^{\frac{2}{5}}$ to satisfy the identity

$$c_1 M h_2^{\frac{5}{2}} = \delta, \tag{3.8}$$

then $||f_k - f_\delta||_{L^2(0,1)} = \delta$, $k = 1, 2$. Thus

$$\gamma^2_{\delta,a} := \inf_{R_{h(\delta)}} \sup_{f\in\mathcal{K}^2_{\delta,a}} ||R_{h(\delta)} f_\delta - f'||_2 \ge \inf_{R_{h(\delta)}} \max_{k=1,2} ||R_{h(\delta)} f_\delta - f_k'||_2$$

$$= \inf_{\varphi\in\mathcal{L}} \max\left\{||\varphi - f_1'||_2, ||\varphi + f_1'||_2\right\},$$

where $\mathcal{L} := \{\varphi : \varphi = cf_1' + \psi, \ \psi \perp f'\}$. Therefore

$$\gamma^2_{\delta,a} \ge \inf_{c\in\mathbb{R},\, \psi\perp f'} \max\left\{\sqrt{(1-c)^2||f_1'||_2^2 + ||\psi||_2^2}, \sqrt{(1+c)^2||f_1'||_2^2 + ||\psi||_2^2}\right\}$$

$$= \inf_{c\in\mathbb{R}} \max\left\{|1-c|||f_1'||_2, |1+c|||f_1'||_2\right\} = ||f_1'||_2$$

$$= c_2 M h_2^{\frac{3}{2}} = c_2 M^{\frac{2}{5}} \left(\frac{\delta}{c_1}\right)^{\frac{3}{5}}. \tag{3.9}$$

If $a = 0$, then (3.8) yields $f_k \in \mathcal{K}^2_{\delta,0}$, $k = 1, 2$, with $N_{0,2} := c_1 M h^{\frac{5}{2}} = \delta$, and one gets $\gamma^2_{\delta,0} \to \infty$ as $M \to \infty$.

Given constants δ and $N_{1,2}$ (in the case $a = 1$), one takes $h = h_2 := \left(\frac{\delta}{c_1 M}\right)^{\frac{2}{5}}$ so that $||f_k - f_\delta||_2 = \delta$, and then takes M so that $C_2 M^{\frac{2}{5}} \left(\frac{\delta}{c_1}\right)^{\frac{3}{5}} = N_{1,2}$. With this choice of h_2 and M the functions $f_k \in \mathcal{K}^2_{\delta,1}$, $k = 1, 2$, and one obtains from (3.9)

$$\gamma^2_{\delta,1} \geq N_{1,2} > 0 \quad \text{as} \quad \delta \to 0. \tag{3.10}$$

Finally, consider $a \in (1, 2)$, $p \geq 1$. For the operator $R_{h(\delta)}$ defined by (1.1) one gets using the Lagrange formula:

$$\begin{aligned} ||R_{h(\delta)} f_\delta - f'||_p &\leq ||R_{h(\delta)}(f_\delta - f)||_p + ||R_{h(\delta)} f - f'||_p \\ &\leq \frac{2\delta}{h} + N_{a,p} h^{a_0}. \end{aligned} \tag{3.11}$$

Minimizing the right-hand side of (3.11) with respect to $h \in (0, \infty)$ yields

$$h_a(\delta) = \left(\frac{2\delta}{a_0 N_{a,p}}\right)^{\frac{1}{a}}, \quad \eta(\delta) = a(N_{a,p})^{\frac{1}{a}} \left(\frac{2\delta}{a_0}\right)^{\frac{a_0}{a}}, \quad a = 1 + a_0, \quad 0 < a_0 < 1.$$

The case $a = 2$ is treated in the introduction (see estimate (1.2)). So one arrives at (2.9)-(2.10). This completes the proof. □

Proof of Theorem 2.2

We give two proofs based on quite different methods.

The first proof uses the construction of the regularizing operator $R_{h(\delta)}$ defined in (1.1). The right-hand side of the error estimate of the type (1.2) is now replaced by $E(h) := \frac{2\delta}{h} + w(h)$, where $w \to 0$ as $h \to 0$, provided that $a = 1$. Minimizing E with respect to h for a fixed δ, one obtains a minimizer $h(\delta) \to 0$ as $\delta \to 0$ and the error estimate $E(h(\delta)) \to 0$ as $\delta \to 0$. Therefore one gets (2.6). Alternatively, if one chooses $h_1(\delta) \to 0$ as $\delta \to 0$, such that $\frac{2\delta}{h_1} = w(h_1)$, then $E(h_1(\delta)) \leq 2w(h_1(\delta)) \to 0$. The first proof is completed. □

Remark 3.1 The statement of Theorem 2.2 with (2.6) replaced by (2.7) is obvious: since f is fixed, one may take $R_{h(\delta)} f_\delta = f'$. This is, of course, of no practical use because f' is unknown.

The second proof is longer, but the ideas of this proof have an advantage of being applicable to a wide variety of ill-posed problems [21], and not only to stable numerical differentiation. By this reason we give this proof in detail ([23]). In order to show that for $a = 1$ there exists an operator $R_{h(\delta)} : L^2(0,1) \to L^2(0,1)$, ($L^2(0,1)$ is a *real* Hilbert space) such that (2.6) holds we will use the DSM (dynamical systems approach) (see [23], [21]). This approach consists of the following steps:

Step 1. Solve the Cauchy problem:

$$\dot{v} = -[Av + h(t)v - f_\delta], \quad v(0) = v_0 \in L^2(0,1), \tag{3.12}$$

where A is defined in (2.2), $p = 2$, $\dot{v} := \frac{dv}{dt}$, $||f_\delta - f|| \le \delta$ and

$$h(t) \in C^1[0,+\infty), \quad h(t) > 0, \quad h(t) \searrow 0, \quad \frac{\dot{h}(t)}{h^2(t)} \to 0 \text{ as } t \to +\infty. \tag{3.13}$$

Step 2. Calculate $v(t_\delta)$, where $t_\delta > 0$ is a number such that $t_\delta \to +\infty$ and $\frac{\delta}{h(t_\delta)} \to 0$ as $\delta \to 0$. Then

$$R_{h(\delta)} f_\delta := v(t_\delta) \tag{3.14}$$

and

$$\sup_{f_\delta \in \mathcal{B}^2_{\delta,f}} ||R_{h(\delta)} f_\delta - f'||_2 \le \eta(\delta, f) \to 0 \text{ as } \delta \to 0 \tag{3.15}$$

with $\eta(\delta, f)$ given by (3.29) below and $f \in \mathcal{K}^2_{\delta,1}$.

To verify (3.15) consider the problem

$$Aw + h(t)w - f = 0. \tag{3.16}$$

Since A is monotone in $L^2(0,1)$:

$$(A\phi, \phi) = \int_0^1 \left(\int_0^x \phi(\tau) d\tau \right) \phi(x) dx = \frac{1}{2} \int_0^1 \left[\left(\int_0^x \phi(\tau) d\tau \right)^2 \right]' dx \ge 0, \tag{3.17}$$

for any $\phi \in L^2(0,1)$ and $h(t) > 0$, the solution $w(t)$ to (3.16) exists, is unique, and admits the estimate

$$(A(w - f'), w - f') + h(t)||w||_2^2 = h(t)(w, f'), \quad ||w||_2 \le \mathcal{N}_{1,2}. \tag{3.18}$$

Differentiate (3.16) with respect to t (this is possible by the implicit function theorem) and get

$$[A + h(t)I]\dot{w} = -\dot{h}(t)w, \quad ||\dot{w}||_2 \le \frac{|\dot{h}(t)|}{h(t)} ||w||_2 \le \frac{|\dot{h}(t)|}{h(t)} \mathcal{N}_{1,2}, \tag{3.19}$$

where (3.18) was used. Denote

$$z(t) := v(t) - w(t). \tag{3.20}$$

From (3.16) and (3.12) one obtains

$$\dot{z}(t) = -\dot{w} - [A + h(t)I]z + f_\delta - f, \quad z(0) = v_0 - w(0). \tag{3.21}$$

Multiply (3.21) by $z(t)$ and get

$$(\dot{z}, z) = -(\dot{w}, z) - (Az, z) - h(t)(z, z) + (f_\delta - f, z). \tag{3.22}$$

Let $||z(t)||_2 := g(t)$, then (3.17) and (3.22) imply

$$g\dot{g} \leq (||\dot{w}||_2 + \delta)g - h(t)g^2. \tag{3.23}$$

Since $g \geq 0$, from (3.23) and (3.19) it follows that

$$\dot{g} \leq \mathcal{N}_{1,2}\frac{|\dot{h}(t)|}{h(t)} + \delta - h(t)g(t), \quad g(0) = ||v_0 - w(0)||. \tag{3.24}$$

So,

$$g(t) \leq e^{-\int\limits_0^t h(s)ds}\left[g(0) + \int\limits_0^t e^{\int\limits_0^\tau h(s)ds}\left(\mathcal{N}_{1,2}\frac{|\dot{h}(\tau)|}{h(\tau)} + \delta\right)d\tau\right]. \tag{3.25}$$

Under assumption (3.13), one has

$$\int\limits_0^\infty h(t)dt = \infty. \tag{3.26}$$

Indeed, (3.13) implies $\frac{|\dot{h}|}{h^2} \leq c$, $c = \text{const} > 0$, so $\frac{d}{dt}\frac{1}{h} \leq c$, $\frac{1}{h(t)} - \frac{1}{h(0)} \leq ct$, $\frac{1}{h(t)} \leq c_0 + ct$, $c_0 := [h(0)]^{-1} > 0$, and $h(t) \geq \frac{1}{c_0+ct}$. Conclusion (3.26) follows.

If one chooses $t = t_\delta$ so that $t_\delta \to +\infty$ and $\frac{\delta}{h(t_\delta)} \to 0$ as $\delta \to 0$, then by (3.25) and (3.26), using L'Hospital's rule one obtains

$$||v(t_\delta) - w(t_\delta)||_2 := g(t_\delta) \to 0 \quad \text{as} \quad \delta \to 0. \tag{3.27}$$

The existence of the solution to (3.12) on $[0, +\infty)$ is obvious, since equation (3.12) is linear with a bounded operator.

We claim that

$$||w(t_\delta) - f'||_2 \to 0 \quad \text{as} \quad \delta \to 0 \tag{3.28}$$

For convenience of the reader this claim is established below. Equations (3.13), (3.25), (3.27), and (3.28) imply:

$$\sup_{f_\delta \in \mathcal{B}^2_{\delta,f}} ||v(t_\delta) - f'||_2 \leq ||w(t_\delta) - f'||_2 + e^{-\int\limits_0^{t_\delta} h(s)ds}\Bigg[g(0)+$$

$$+\int\limits_0^{t_\delta} e^{\int\limits_0^\tau h(s)ds}\left(\mathcal{N}_{1,2}\frac{|\dot{h}(\tau)|}{h(\tau)} + \delta\right)d\tau\Bigg] := \eta(\delta, f) \to 0 \quad \text{as} \quad \delta \to 0. \tag{3.29}$$

Let us now prove (3.28). Because $f' \in L^2(0,1)$ and $f(0) = 0$, one can rewrite (3.16) as $A(w - f') + h(t)w = 0$. This and the monotonicity of A imply $h(t)(w, w - f') \leq 0$, so, since $h(t) > 0$, one gets $(w, w - f') \leq 0$, and $||w||_2 \leq ||f'||_2$. Thus w converges weakly in $L^2(0,1)$ to some element ψ, $w \rightharpoonup \psi$ as $t \to \infty$. Because A is monotone, it is weakly closed, that is $w \rightharpoonup \psi$ and $A(w - f') \to 0$ imply $A(\psi - f') = 0$, so $\psi = f'$ and $w \rightharpoonup f'$. The inequality $(w, w - f') \le 0$ can be written as $||w - f'||_2^2 \le (f', f' - w)$, and $(f', w - f') \to 0$ because $w - f' \rightharpoonup 0$. Therefore the claim is proved and the second proof is completed. □

4. Numerical Aspects

Figures 1-4 illustrate the impossibility to differentiate stably a function, which does not have a bound on $f^{(a)}$, $a > 1$. If one takes the function

$$f(x) := \begin{cases} \frac{\mathcal{N}_{1,\infty}^2}{4\delta} x(x - \frac{4\delta}{\mathcal{N}_{1,\infty}}), & 0 \le x \le 4\delta \\ 0, & 4\delta < x \le 1, \end{cases} \tag{4.1}$$

and $f_\delta \equiv 0$, then

$$f(x) \in \{f :\ f \in W^{1,\infty}(0,1),\ ||f'||_\infty < \mathcal{N}_{1,\infty},\ ||f - f_\delta||_\infty \le \delta\},$$

and any formula of numerical differentiation will give error not going to zero as $\delta \to 0$, because, by (3.6), one has:

$$\inf_{R_h(\delta)} ||R_h(\delta) f_\delta - f'||_\infty \ge \mathcal{N}_{1,\infty}.$$

In Figure 1 one can see $f(x)$ given by (4.1) with $\delta = 0.1$ and $\mathcal{N}_{1,\infty} = 1$:

$$f(x) := \begin{cases} 2.5x(x - 0.4), & 0 \le x \le 0.4 \\ 0, & 0.4 < x \le 1. \end{cases} \tag{4.2}$$

Figure 2 presents

$$f'(x) := \begin{cases} 5x - 1, & 0 \le x \le 0.4 \\ 0, & 0.4 < x \le 1. \end{cases} \tag{4.3}$$

Figure 3 shows the case $\delta = 0.01$ and $\mathcal{N}_{1,\infty} = 0.5$:

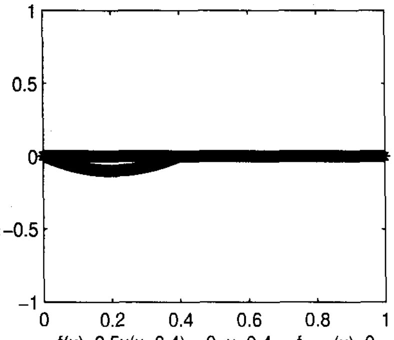
$$f(x) := \begin{cases} 6.25x(x - 0.08), & 0 \le x \le 0.08 \\ 0, & 0.08 < x \le 1. \end{cases} \tag{4.4}$$

The derivatives are given in Figure 4:

$$f'(x) := \begin{cases} 12.5x - 0.5, & 0 \le x \le 0.4 \\ 0, & 0.4 < x \le 1. \end{cases} \tag{4.5}$$

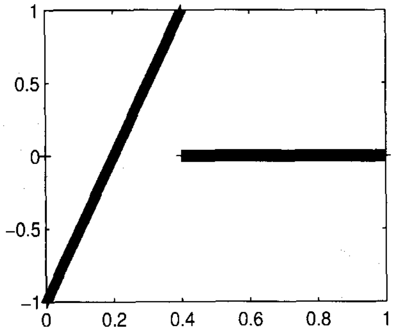
Even if the bound on $f^{(a)}$ in some norm is given, one can experience difficulties with stable differentiation. Namely, if δ is fixed and $\mathcal{N}_{a,p}$ is very large, then h_{opt} in finite difference scheme (1.1) is very small, and practitioners might not have sufficiently many observation points. Another difficulty is: the estimated error $\varepsilon_{a,p}$ in such a case is very big and does not give any information regarding the accuracy of computations. This is illustrated in Table 1 below for the function $f(x) = \sin((\pi x)^n)$ and $\delta = 0.1$.

Figure 1



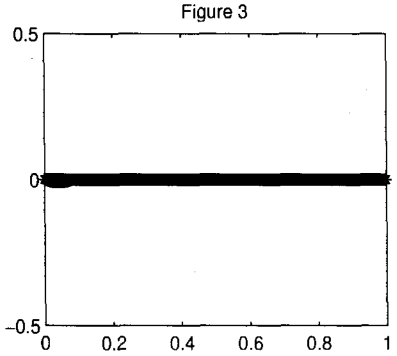
f(x)=2.5x(x−0.4), 0<x<0.4, f_{delta}(x)=0

Figure 2



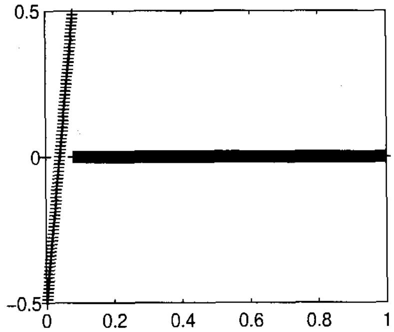
f'(x)=5x−1, 0<x<0.4

Figure 3



f(x)=6.25x(x−0.08), 0<x<0.08, f_{delta}(x)=0

Figure 4



f'(x)=12.5x−0.5, 0<x<0.08

Table 1.

n	$\mathcal{N}_{2,p}$	h_{opt}	$\varepsilon_{a,p}$
5	$1.24 \cdot 10^{6}$	$5.67 \cdot 10^{-4}$	$7.04 \cdot 10^{2}$
10	$3.27 \cdot 10^{11}$	$1.11 \cdot 10^{-6}$	$3.62 \cdot 10^{5}$
15	$4.41 \cdot 10^{16}$	$3.01 \cdot 10^{-9}$	$1.33 \cdot 10^{8}$
20	$7.94 \cdot 10^{21}$	$7.10 \cdot 10^{-12}$	$5.63 \cdot 10^{10}$
25	$2.62 \cdot 10^{27}$	$1.24 \cdot 10^{-14}$	$3.24 \cdot 10^{13}$

Figure 5

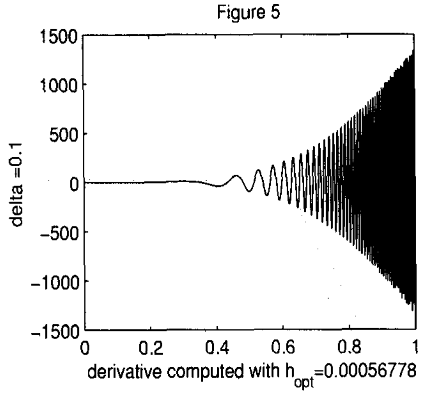


Figure 6

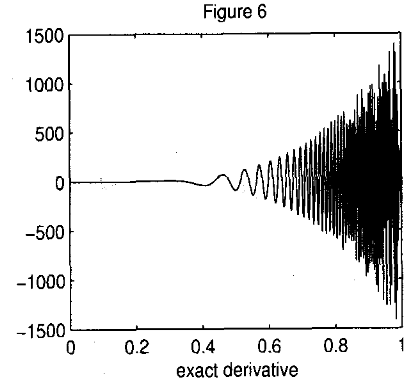


Figure 7

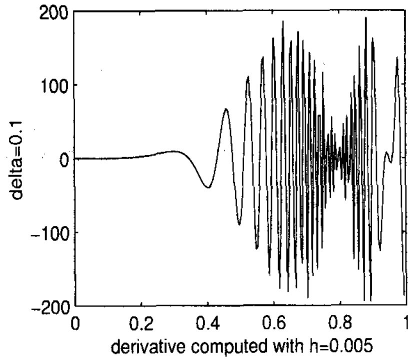
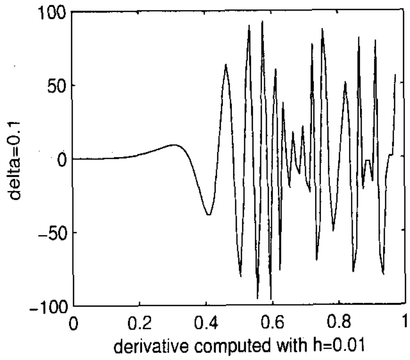


Figure 8



Figures 5-8 show the exact and computed derivatives of $f(x) = \sin((\pi x)^5)$. The derivatives of this function were computed in the presence of the noise function

$$e(x) = \delta(\cos(2x) + \cos(3x^2))/2, \tag{4.6}$$

and with different step sizes. One can see in Figure 5 that for h_{opt} the computed derivative is very accurate. However as h grows, the accuracy decreases.

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