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ON STABLE NUMERICAL DIFFERENTIATION

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ABSTRACT. Based on a regularized Volterra equation, two different approaches for numerical differentiation are considered. The first approach consists of solving a regularized Volterra equation while the second approach is based on solving a discretized version of the regularized Volterra equation. Numerical experiments show that these methods are efficient and compete favorably with the variational regularization method for stable calculating the derivatives of noisy functions.

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1. INTRODUCTION

Calculating the derivatives of noisy functions is of prime importance in many applications. The problem consists of calculating stably the derivative of a smooth function f given its noisy data f_δ , $\|f_\delta - f\| \leq \delta$. This is an ill-posed problem: a small error in f may lead to a large error in f' . Many methods have been introduced in the literature. A review is given in [7]. Divided differences method with $h = h(\delta)$ has been first proposed in [4], see also [5, 6, 7]. Necessary and sufficient conditions for the existence of a method for stable differentiation of noisy data are given in [8, chapter 15], see also [9]. In our paper a method for stable differentiation based on solving the regularized Volterra equation

$$(1.1) \quad Au(x) + f_\delta(0) := \int_0^x u(s)ds + f_\delta(0) = f_\delta(x),$$

is proposed (see also [10, 1, 9]). One often applies the Variational Regularization (VR) method

$$(1.2) \quad \|Au - f_\delta\|^2 + \alpha\|u\|^2 \rightarrow \min$$

for stable differentiation.

In this paper (and in [1]) an approach, based on the fact that the quadratic form of the operator A is nonnegative in real Hilbert space $L^2(0, a)$, $a = \text{const} > 0$, is used.

2. METHODS

Consider two different approaches to solving equation (1.1). The first approach consists of solving directly regularized equation (1.1). The second approach is based on the Dynamical Systems method (DSM) and an iterative scheme from [3].

2.1. First method. In [1], the derivatives of a noisy function f_δ are obtained by solving the equation

$$(2.1) \quad \alpha u_{\alpha, \delta} + Au_{\alpha, \delta} = f_\delta.$$

If $\alpha = \alpha(\delta) > 0$ is continuous on $[0, \delta_0)$, $\delta_0 > 0$ and

$$(2.2) \quad \lim_{\delta \rightarrow 0} \alpha(\delta) = 0, \quad \lim_{\delta \rightarrow 0} \frac{\delta}{\alpha(\delta)} = 0,$$

then the following result holds (see [1]):

Theorem 2.1. *Assume (2.2). Then*

$$\lim_{\delta \rightarrow 0} \|u_\delta - u\| = 0,$$

where u_δ solves (2.1) with $\alpha = \alpha(\delta)$.

The solution of (2.1) is:

$$(2.3) \quad u_\delta(x) = -\frac{1}{\alpha^2} \exp\left(-\frac{x}{\alpha}\right) \int_0^x \exp\left(\frac{s}{\alpha}\right) f_\delta(s) ds + \frac{f_\delta(x)}{\alpha}.$$

This formula and an *a priori* choice $\alpha(\delta) = \delta^k/c$, where $k \in (0, 1)$, c is a constant, yield a scheme for stable differentiation. When $\alpha(\delta)$ is known, the problem is reduced to calculating integral (2.3). There are many methods for calculating accurately and fast integral (2.3) (see e.g. [2]). However, there is no known algorithm for choosing k, c which are optimal in some sense. The advantage of our approach is that the CPU time for the method is very small compared with the VR and DSM, see Section 3.1. Moreover, one can calculate the solution analytically when the function f_δ is simple by using tables of integrals or MAPLE.

2.2. An iterative scheme of DSM for solving discretizations of the regularized Volterra equation. Another approach to stable differentiation is to use the DSM (see [8]). The DSM yields a stable solution of the equation:

$$(2.4) \quad F(u) = Au - f = 0, \quad u \in H,$$

where H is a Hilbert space and A is a linear operator in H which is not necessarily bounded but closed and densely defined. The DSM to solve (2.4) is of the form:

$$(2.5) \quad u' = -u + (T + a(s))^{-1}A^*f, \quad u(0) = u_0,$$

where $T := A^*A$ and $a(t) > 0$ is a nonincreasing function such that $a(t) \rightarrow 0$ as $t \rightarrow \infty$. The unique solution to (2.5) is given by

$$(2.6) \quad u(t) = u_0e^{-t} + e^{-t} \int_0^t e^s(T + a(s))^{-1}A^*f ds.$$

An iterative scheme for computing $u(t)$ in (2.6) is proposed in [3]:

$$u_{n+1} = e^{-h_n}u_n + (1 - e^{-h_n})(T + a_n)^{-1}A^*f_\delta, \quad h_n = t_{n+1} - t_n.$$

With a_0 satisfying

$$(2.7) \quad \delta < \|Au_{a_0} - f_\delta\| < 2\delta,$$

one chooses a_n and h_n as follows:

$$a_n = \frac{a_0}{1 + t_n}, \quad h_n = q^n,$$

where $1 \leq q \leq 2$, $t_0 = 0$. To increase the speed of computing we recommend choosing $q = 2$. At each iteration one checks if

$$(2.8) \quad 0.9\delta \leq \|Au_n - f_\delta\| \leq 1.001\delta.$$

This is a stopping criterion of discrepancy principle type (see [3]). If t_n is the first time such that (2.8) is satisfied, then one stops and takes u_n as the solution to (2.4). The choice of a_0 satisfying (2.7) is done by iterations as follows:

- (1) As an initial guess for a_0 one takes $a_0 = \frac{1}{3}\|A\|^2\delta_{rel}$, where $\delta_{rel} = \frac{\delta}{\|f\|}$.
- (2) If $\frac{\|Au_{a_0} - f_\delta\|}{\delta} = c > 3$, then one takes $a_1 := \frac{a_0}{2(c-1)}$ as the next guess and checks if condition (2.8) is satisfied. If $2 < c \leq 3$ then one takes $a_1 := a_0/3$.
- (3) If $\frac{\|Au_{a_0} - f_\delta\|}{\delta} = c < 1$, then $a_1 := 3a_0$ is used as the next guess.
- (4) After a_0 is updated, one checks if (2.8) is satisfied. If (2.8) is not satisfied, one repeats steps 2 and 3 until one finds a_0 satisfying condition (2.8).

Algorithms for choosing a_0 and computing u_n are detailed in algorithms 1 and 2 in [3].

3. NUMERICAL EXPERIMENTS

Numerical experiments are carried out in MATLAB in double-precision arithmetic. In all experiments, by $u(t)$, $u_{[1]}(t)$, $u_{DSM}(t)$ and $u_{VR}(t)$ we denote the exact derivative, the derivatives computed by the first, the DSM and the VR methods, respectively. In this section by n we denote the number of points used to discretize the interval $[0, 1]$.

3.1. Computing the first derivatives of a noisy function. Let us compute the derivatives of the function $f(t) = \sin(\pi t)$ contaminated by the noise function $e(t) = \delta \cos(10\pi t)$. The derivative of $f(t)$ is $f'(t) = \pi \cos(\pi t)$. To solve this problem we use three methods: the first method, based on computing integral (2.3), the VR method, and the DSM method, based on a discretized version of (1.1). Numerical results for this problem are presented in Figure 1. In our experiments, since the results obtained by the DSM and the VR are nearly the same, we present only the results for the DSM in Figure 1 and 2 in order to make these figures simple.

In this experiment the trapezoidal quadrature rule is applied to integral equation (1.1) and is used for computing integral (2.3). One may use higher order interpolation methods to compute integral (2.3). However, it does not necessarily bring improvements in accuracy. This is so because using a high order interpolation method for inaccurate data may even lead to worse results. This is the case when the noise level is large.

The approximate derivative formula (2.3) for t close to 0 does not use much information about f_δ . Thus, we only use (2.3) for computing $f'(t)$ for $t \in [\frac{1}{2}, 1]$. For $t \in [0, \frac{1}{2})$, we take $g_\delta(t) := f_\delta(1-t)$ and use formula (2.3) for $g_\delta(t)$ with $t \in (\frac{1}{2}, 1]$. That is, we have a discontinuity at $t = \frac{1}{2}$ of the solution, obtained by the first method in Figure 1 and 2. The same idea is applied in discretizing equation (1.2) in the implementation of the DSM and VR.

In the DSM and VR we also use the trapezoidal quadrature rule to discretize equation (1.1). Since the right-hand side f_δ contains noise, using high order collocation methods does not necessarily improve the accuracy. Experiments have shown that the use of higher order collocation methods leads to linear algebraic systems with larger condition numbers and yields numerical solutions with lower accuracy.

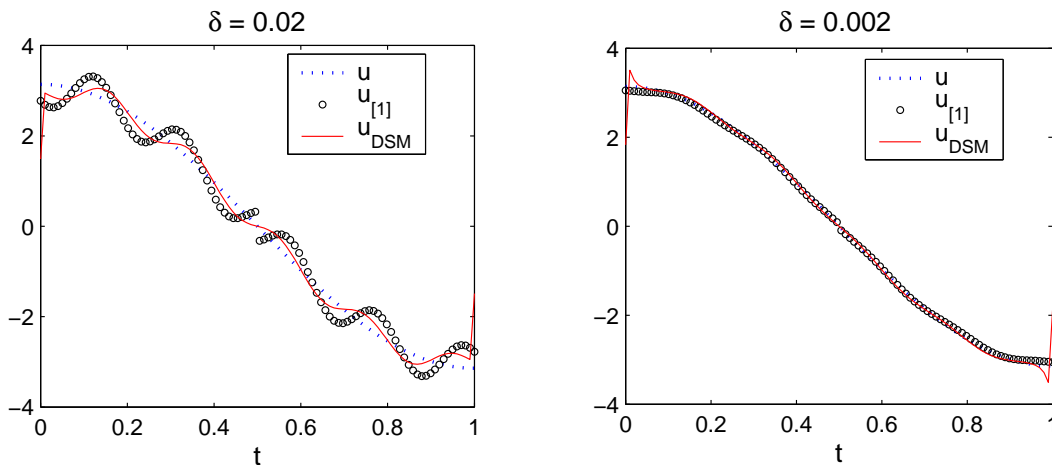


Figure 1: Numerical results for $f_\delta(x) = \sin(\pi t) + \delta \cos(10\pi t)$. Discretization points $n = 100$.

The CPU times for the VR and DSM are about 0.0125 sec. The CPU time for the first method is much smaller: 0.0015 sec. Here, we should bear in mind that the DSM and the VR use iterations to look for "good" regularization parameter α while the code based on the first method does nothing to look for α but uses α as an input value. If one also uses the regularization parameter as an input in the VR and DSM, although these methods still take more time than the first method the difference in computation time is not so large.

The error of the first method for $\delta = 0.02$ is larger than those of the VR and the DSM, but when $\delta = 0.002$ then the first method gives smaller errors. From Figure 1 and 2, one can see

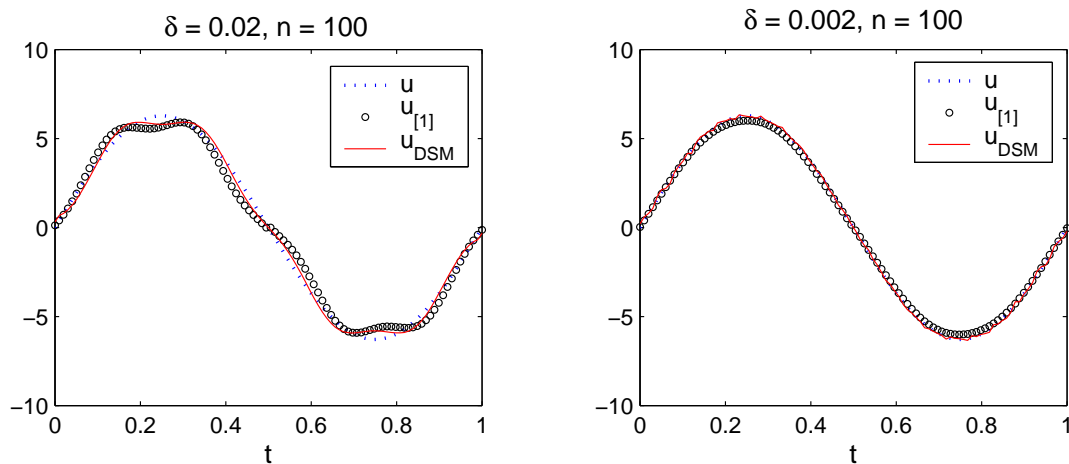


Figure 2: Numerical results for $f_\delta(x) = \sin(2\pi t - \frac{1}{2}\pi) + \delta \cos(10\pi t)$. Discretization points $n = 100$.

that the solutions obtained by the DSM are better than those obtained by the first method for all $t \in [0, 1]$ except for the t which are close to the boundary of the interval. Indeed, it can be showed analytically that the solution u to equation (1.2) satisfies $u(0) = u(1) = 0$. However, the derivative of f in Figure 1 satisfies $f'(0) = \pi$ and $f'(1) = -\pi$. If the computed derivatives at the points close to the boundary are discarded, then in both cases the DSM and the VR are more accurate than the first method.

Figure 2 presents the numerical experiment for $f(t) = \sin(2\pi t - \frac{1}{2}\pi)$ contaminated by the same noise function $e(t) = \delta \cos(10\pi t)$. For this problem, since the function to be differentiated f satisfies $f'(0) = f'(1) = 0$ both the DSM and the VR give more accurate results than the first method.

From Figure 1 and 2 one can see that for $\delta = 0.02$ the computed derivatives are very close to the exact derivative at all points except for those close to the boundary in Figure 1.

3.2. Computing the second derivatives of a noisy function. Let us give numerical results for computing the second derivatives of noisy functions. The problem is reduced to an integral equation of the first kind. A linear algebraic system is obtained by a discretization of the integral equation whose kernel K is Green's function

$$K(s, t) = \begin{cases} s(t-1), & \text{if } s < t \\ t(s-1), & \text{if } s \geq t \end{cases}.$$

Here $s, t \in [0, 1]$ and as the right-hand side f and the corresponding solution u one chooses one of the following (see [3]):

$$\text{case 1, } f(s) = \frac{s^3 - s}{6}, \quad u(s) = s, \quad 0 \leq s \leq 1,$$

$$\text{case 2, } f(s) = \frac{\sin(2\pi s)}{4\pi^2} + s - 1, \quad u(s) = \sin(2\pi s), \quad 0 \leq s \leq 1.$$

Collocation method is used for discretization. This discretization can be improved by other methods but we do not go into detail. We use $n = 10, 20, \dots, 100$, and $b_{n,\delta} = b_n + e_n$, where e_n is a vector containing random entries, normally distributed with mean 0, variance 1, and scaled so that $\|e_n\| = \delta_{rel} \|b_n\|$. This linear algebraic system is mildly ill-posed: the condition number of A_{100} is 1.2158×10^4 .

Case 1					Case 2				
n	DSM		VR		n	DSM		VR	
	N_{insol}	$\frac{\ u_\delta - y\ _2}{\ y\ _2}$	N_{insol}	$\frac{\ u_\delta - y\ _2}{\ y\ _2}$		N_{insol}	$\frac{\ u_\delta - y\ _2}{\ y\ _2}$	N_{insol}	$\frac{\ u_\delta - y\ _2}{\ y\ _2}$
20	3	0.3319	5	0.3440	20	4	0.0773	4	0.0780
40	4	0.3206	6	0.3253	40	3	0.0484	6	0.0520
60	4	0.3264	6	0.3312	60	4	0.0355	6	0.0438
80	4	0.3019	7	0.3014	80	3	0.0407	5	0.0479
100	5	0.2956	7	0.2948	100	4	0.0254	6	0.0379

Table 3.1: Results for case 1 and 2 with $\delta_{rel} = 0.01$, $n = 20, 40, \dots, 100$.

Table 3.1 shows that numerical results obtained by the DSM are more accurate than those by the VR. Figure 3 plots the numerical solutions for these cases. The computation time of the DSM in these cases is about the same as or less than that of the VR. From Table 3.1 one can see that both the DSM and the VR perform better in case 2 than in case 1. Note that the regularized equation to solve for second derivatives in this case is of the same form as equation (1.2). As we discussed earlier, it is because in case 2 we have $f'(0) = f'(1) = 0$.

We conclude that in this experiment the DSM competes favorably with the VR.

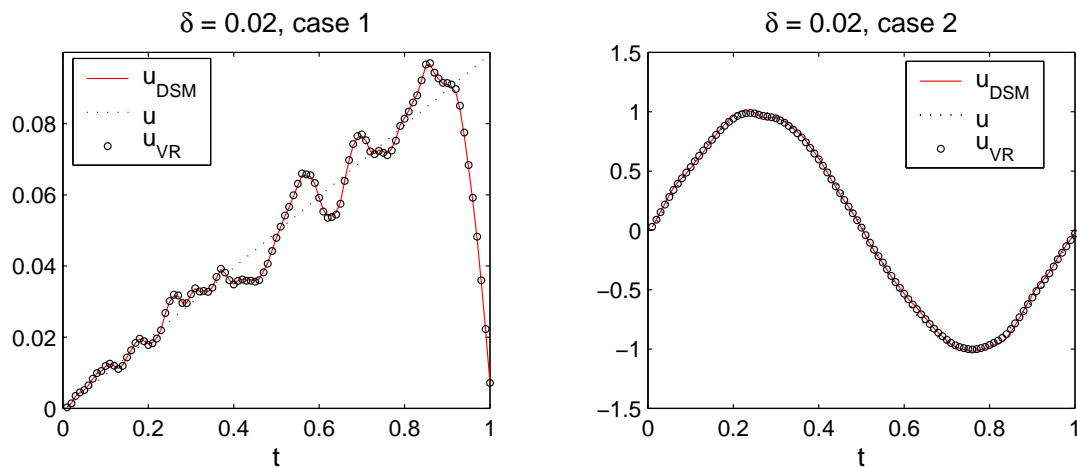


Figure 3: Plots of solutions obtained by DSM, VR when $n = 100$, $\delta_{rel} = 0.02$.

Looking at Figure 3 case 1, one can see that the computed values at $t = 0$ and $t = 1$ are zeros. Again, the regularized scheme forces the computed derivative u to satisfy the relations $u(1) = u(0) = 0$. If one wants to compute the derivative of a noisy function on an interval by the proposed method, one should collect data on a larger interval and use this method to calculate the derivative at the points which are not close to the boundary.

4. CONCLUDING REMARKS

In this paper two approaches to stable differentiation of noisy functions are discussed. The advantage of the first approach is that it contains neither matrix inversion nor solving of linear algebraic systems. Its computation time is very small. The drawback of the method is that there is no known *a posteriori* choice of $\alpha(\delta)$. The second approach is an implementation

of the DSM. It competes favorably with the VR in both computation time and accuracy. The DSM competes favorably with the VR in solving linear ill-conditioned algebraic systems. A *posteriori* choice of α , an efficient way to compute integral (2.3) for the first method, and an efficient discretization of the Volterra equation (1.1) with the implementation of the DSM are planned for future research.

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