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SENSITIVITY VIA THE COMPLEX-STEP METHOD FOR DELAY DIFFERENTIAL EQUATIONS WITH NON-SMOOTH INITIAL DATA

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Abstract. In this report, we use the complex-step derivative approximation technique to compute sensitivities for delay differential equations (DDEs) with non-smooth (discontinuous and even distributional) history functions. We compare the results with exact derivatives and with those computed using the classical sensitivity equations whenever possible. Our results demonstrate that the implementation of the complex-step method using the method of steps and the Matlab solver dde23 provides a very good approximation of sensitivities as long as discontinuities in the initial data do not cause loss of smoothness in the solution: that is, even when the underlying smoothness with respect to the initial data for the Cauchy-Riemann derivation of the method does not hold. We conclude with remarks on our findings regarding the complex-step method for computing sensitivities for simpler ordinary differential equation systems in the event of lack of smoothness with respect to parameters.

1. Introduction. Sensitivity analysis is of interest in widely diverse topics in mathematics and engineering including parameter selection and identifiability (see [9] and the

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references therein), inverse problem formulations [4,8], optimal design [12,13] among others. In this wide range of applications, sensitivities may be desired for model problems coming from real world applications. Often in such cases one encounters non-smooth problems where one does not have analyticity of the response with respect to parameters. Such problems include sensitivity analysis of delay systems with respect to delays (our focus in this note) where in general the solution may lack smoothness in initial histories [14]; PDE problems and sensitivity with respect to boundary parameters (our initial motivation for our investigations of the complex-step methods; see [5]), and sensitivities in aggregate data problems where estimated parameters are probability measures [10, Chapter 6].

Delay equations have been used in a wide variety of biological applications as well as in many engineering problems; see for examples the references [1–3, 6, 7, 16–19, 22]. Early applications of delay differential equations date back to the 1940s for studies of mechanical systems by Minorsky [27–29] and slightly later for studies of population dynamics in biology by Hutchinson [20, 21]. Delay differential equations (DDEs) are particularly interesting because the derivatives of their solutions often have discontinuities (see [14] for a theoretical treatment and discussions). This is generally true because the first derivative of a non-constant history function at zero is almost always different from the right derivative of the solution at the initial point. As we shall see below, in addition to the discontinuity at the initial point, discontinuities in derivatives of the initial function tend to be propagated with one degree of smoothness added per time delay interval. Since the complex-step method is derived assuming analyticity, one might expect for the method to fail when it comes to computing the sensitivity with respect to the time lag τ. But the results for these examples show that the complex-step method approximates the sensitivities accurately up to a critical step size (h_{crit}) in certain cases even in lack of smoothness with respect to the parameters.

In sensitivity analyses, we study how the output of a model is affected by its inputs such as parameters and initial data. Hence, we are concerned with calculating the rates of change in the output variables (solutions or observables) of a system which result from small perturbations in the problem parameters λ. A major source of these problems involve inverse problems or estimation problems. Following an ODE inverse problem framework, we outline the basic ideas which arise even if we are concerned with delay differential equations (DDEs) where the delays are viewed as parameters to be varied and ultimately to be estimated. Consider an n-dimensional vector system

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{g}(t, \mathbf{x}(t), \mathbf{q}) \\ \mathbf{x}(t_0) &= \mathbf{x}_0 \end{aligned} \tag{1.1}$$

with observation process (we assume without loss of generality a scalar observation process)

$$f(t; \boldsymbol{\lambda}) = C\mathbf{x}(t; \boldsymbol{\lambda}),$$

where $\boldsymbol{\lambda} = [\mathbf{q}^{\mathsf{T}}, {\mathbf{x}_0}^{\mathsf{T}}]^{\mathsf{T}}$, and $\mathbf{q}$ is a vector of length p so that $\boldsymbol{\lambda}$ is a vector of length $p + n$. The inverse problem is to determine $\boldsymbol{\lambda}$ using given observations over time. Using an ordinary least-squares method (OLS) corresponding to an error model $Y_j = f(t_j; \boldsymbol{\lambda}) + \mathcal{E}_j$

(where the $\mathcal{E}_j$ are normally distributed with mean zero and variance σ_0^2) for estimation (more general formulations can be found in [10, 15]), we wish to find

$$\hat{\boldsymbol{\lambda}}_{\text{OLS}} = \arg \min_{\boldsymbol{\lambda} \in \Omega_{\boldsymbol{\lambda}}} \sum_{j=1}^{n} (y_j - f(t_j; \boldsymbol{\lambda}))^2$$

where y_j is the data (a realization of Y_j) at times t_j and $\Omega_{\boldsymbol{\lambda}}$ is the admissible set for the parameters. Using asymptotic properties of estimators ([10, 15]), it can be shown the estimator (a random variable) $\boldsymbol{\lambda}_{\text{OLS}}$ (for which $\hat{\boldsymbol{\lambda}}_{\text{OLS}}$ is a realization) can be approximated (as $n \to \infty$) by a normal distribution with mean $\boldsymbol{\lambda}_0$ (the so-called "true" or nominal parameters) and covariance matrix $\Sigma_0 \approx \sigma_0^2 [\chi^T \chi]^{-1}$ where

$$\chi_{jk} = \frac{\partial f(t_j; \boldsymbol{\lambda})}{\partial \lambda_k}. \tag{1.2}$$

The matrix χ is called the *sensitivity matrix*. The goal is to compute the essential *sensitivities* $\frac{\partial f(t_j;\boldsymbol{\lambda})}{\partial \lambda_k}$ as efficiently and accurately as possible. There are various ways of approximating these derivatives (see [5, 10, 11, 15] and the references therein for survey and comparison of different techniques).

More recently, a method referred to as *the complex-step* has gained some popularity in calculating sensitivities ([25, 26]). The idea of using complex variables to estimate derivatives originated with the work of Lyness and Moler [24] and Lyness [23]. The complex-step estimate is suitable for use in numerical computing and shown in general to be very accurate, extremely robust while retaining a reasonable computational cost. See [25] for extensive discussion of the method and [5] for applications of the method to various problems.

In this report, we apply the complex-step method to compute sensitivities for delay differential equations that have discontinuities in their history functions (initial data) and, in some cases, when this history function is a generalized function which results in discontinuity in the solution itself after the initial time (e.g., see Example 4 below).

2. The complex-step derivative approximation technique.

In this section, we follow [5] and [25], and summarize the complex-step method.

If f is a real function of a real variable and analytic (an assumption we wish to demonstrate is not necessary for the method to work well), we have a Taylor series expansion

$$f(q + ih) \approx f(q) + ihf'(q) - \frac{h^2}{2!} f''(q) - i\frac{h^3}{3!} f^{(3)}(q) + \frac{h^4}{4!} f^{(4)}(q) + \cdots,$$

taking the imaginary parts of both sides and dividing by h results in the first order approximation

$$\frac{df}{dq} = f'(q) \approx \frac{\text{Im}[f(q + ih)]}{h} \tag{2.1}$$

with a truncation error E_T given by

$$E_T(h) = \frac{h^2}{6} f^{(3)}(q).$$

Equation (2.1) can also be derived using the Cauchy-Riemann equations for analytic functions (see [5] and [25]) or a Taylor series with remainder approach in the event of less smoothness in solutions; see our discussions below.

Implementation steps

(1) Define all functions and operators that are not defined for complex arguments. For example *max, min*, *abs* and *transpose.*

(2) Add a small complex step ih to the desired variable 'q', run the algorithm that evaluates f.

(3) Compute df/dq using (2.1):

$$\frac{\partial f}{\partial q} \approx \frac{\mathrm{Im}[f(q+ih)]}{h}.$$

We illustrate the procedure using a general delay differential model with discrete delay as follows:

$$\frac{dx}{dt}(t) = F(t, x(t), x(t-\tau)),\ t \in [0, T], \tag{2.2}$$

$$z(\theta) = x(\theta) = \begin{cases} \phi(\theta), & -\tau \leq \theta < 0, \\ x_0, & \theta = 0, \end{cases} \tag{2.3}$$

where $z_0 = (x_0, \phi) \in \mathbb{R} \times L^2(-\tau, 0; \mathbb{R})$. The resulting state space formulation can be properly formulated in $Z = \mathbb{R} \times L^2(-\tau, 0; \mathbb{R})$ with elements $z(t) = (x(t), x_t)$ where $x(t) = x(t; z_0, \tau) \in \mathbb{R}, x_t(\xi) = x(t+\xi), \xi \in [-\tau, 0]$. Here we are interested in the parameter $q = \tau$ and hence $\frac{\partial x}{\partial \tau}$, where in some cases the solution $x(t; z_0, \tau)$ may not be smooth in τ (e.g., see [14]). We formulate this in a 2-step procedure.

STEP 1. For a given small step size h, solve the system (2.2) with τ replaced by $\tau + ih$, i.e., solve

$$\frac{dx}{dt}(t) = F(t, x(t), x(t-(\tau+ih))),\ t \in [0, T], \tag{2.4}$$

$$x(\theta) = \begin{cases} \phi(\theta), & -\tau \leq \theta < 0, \\ x_0, & \theta = 0. \end{cases} \tag{2.5}$$

STEP 2. Compute the derivative $\partial x/\partial \tau$ using the formula

$$\frac{\partial x}{\partial \tau}(t) \approx \frac{\mathrm{Im}[x(t; \tau+ih)]}{h}. \tag{2.6}$$

3. Numerical examples. In this section we consider a series of examples for which the usual underlying foundations for derivation of the complex-step method do not hold. In particular, we consider *delay differential equations (DDEs)* where sensitivity with respect to the delays or hysteresis kernels do *not* in general satisfy the analyticity requirements for use of the Cauchy-Riemann equations (as required in the derivation of [23, 24]) or an analytic expansion.

For all our examples, we consider the delay differential equations of the form:

$$\frac{dx}{dt}(t) = x(t-\tau; \tau),\ t \in (0, T], \tag{3.1}$$

$$x(\theta) = \phi(\theta), \quad \theta \in [-\tau, 0], \tag{3.2}$$

where the history function ϕ is a discontinuous function. As usual we require that solutions satisfy (3.1) for almost every t and the initial conditions (3.2) for each $\theta \in [-\tau, 0]$. We compute sensitivity to delay $(dx/d\tau)$ using the complex-step derivative approximation technique. We typically let τ be 1. The results are compared whenever possible with exact derivatives and derivatives obtained using sensitivity equations as derived in [10, 15].

In the first two examples we show that when irregularities in the initial data result in lack of regularity in the solutions, the complex-step implementation fails to approximate the sensitivities accurately. The third example demonstrates that if a discontinuous initial data produces a continuous solution in terms of the sensitivity parameter, the complex-step approximates the sided derivatives accurately.

In the fourth example we look at a distribution initial data which results in a jump discontinuity in the solution. In this example we see that, even though there is a jump in the solution, as long as the sided derivatives exist and are equal, the complex-step approximates the sensitivities accurately up to the jump.

For all computations we use the method of steps and Matlab solver dde23 [30] after modifications according to Section 2. And throughout we use a step size $h = 10^{-40}$ for the complex-step approximation of the derivatives. We also take $T = \tau = 1$ in our studies.

Example 1. We consider first an example with a jump discontinuity in the initial data which produces a continuous but not continuously differentiable (with respect to either t or τ) at $t = \frac{1}{2}$.

$$\frac{dx}{dt}(t) = x(t-\tau;\tau), \tag{3.3}$$

$$x(\theta) = \phi(\theta) = \begin{cases} -\theta - 1/2, & -\tau \le \theta < -\tau/2, \\ -\theta, & -\tau/2 \le \theta \le 0. \end{cases} \tag{3.4}$$

The solution for this system is:

$$x(t) = \begin{cases} -\frac{t^2}{2} + \tau t - \frac{1}{2}t & \text{for} \quad 0 \le t < \tau/2, \\ -\frac{t^2}{2} + \tau t - \frac{1}{4}\tau & \text{for} \quad \tau/2 \le t \le \tau, \end{cases} \tag{3.5}$$

and the exact derivative $\frac{dx}{d\tau}$ is given by

$$\frac{dx}{d\tau}(t) = \begin{cases} t & \text{for} \quad 0 \le t < \tau/2, \\ t - \frac{1}{4} & \text{for} \quad \tau/2 < t \le \tau. \end{cases} \tag{3.6}$$

– For comparing the results, we also compute $\frac{\partial x}{\partial \tau}$ by solving the sensitivity equations (see description in [5] and the references therein). To derive the sensitivity equations, we let $s(t) = \frac{\partial x(t)}{\partial \tau}$ and differentiate both sides of equation (3.3) with respect to the delay τ, and obtain the following system of sensitivity equations:

$$\frac{ds}{dt}(t) = -\dot{x}(t-\tau) + s(t-\tau), \ t > 0,$$
$$s(\theta) = 0, \quad -\tau \le \theta \le 0,$$

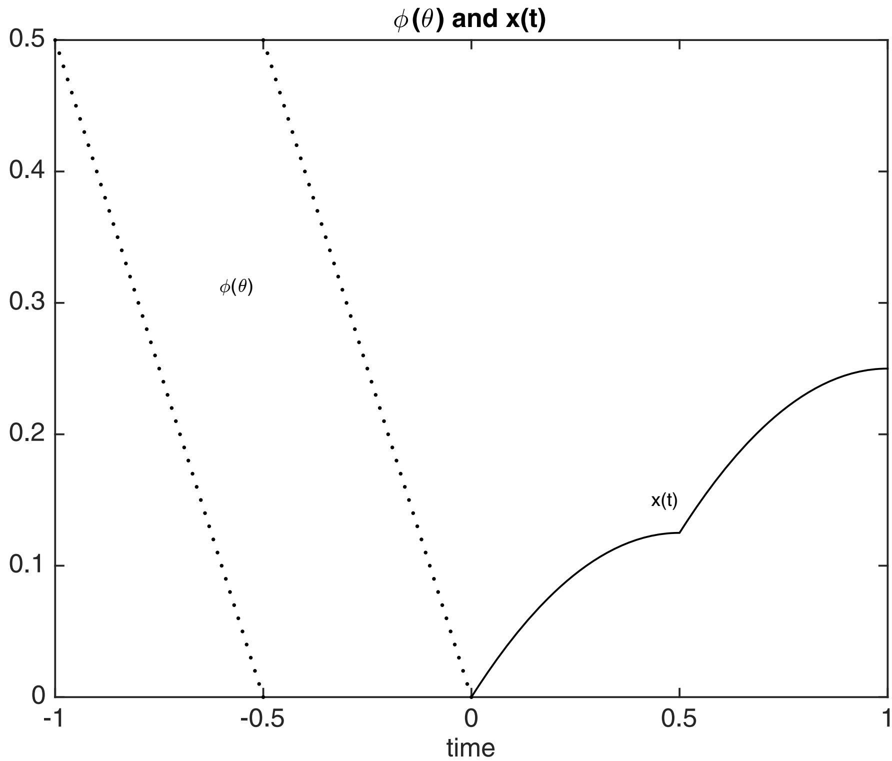


FIG. 1. History and solution functions for DDEs in Example 1 for $\tau = 1$.

where

$$\dot{x}(t-\tau) = -1 \quad \text{for} \quad t \in (0, \tau/2) \cup (\tau/2, \tau).$$

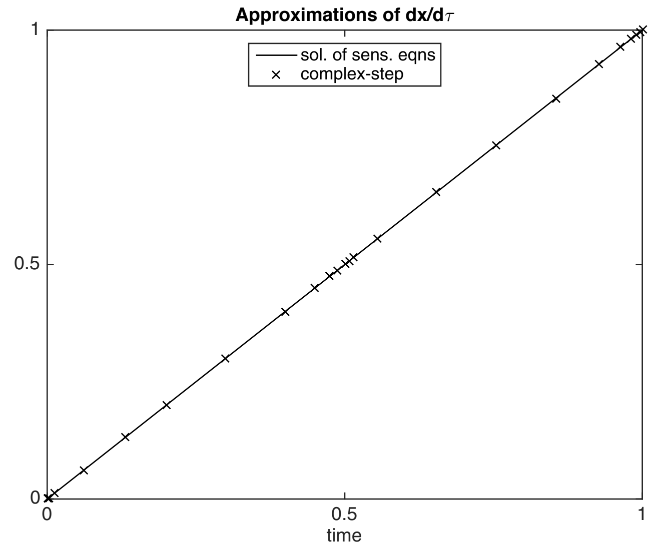
The system is not well defined for $t \in [0, \tau)$ as $s(\tau/2)$ and $\dot{x}(-\tau/2)$ is not defined. This can be seen from the exact derivative given in equation (3.6) and Figure 2 (bottom).

– To compute $\frac{\partial x}{\partial \tau}$ using the complex-step method, first we solve equation (3.3) by replacing τ with $\tau + ih$ for the step size h; then we use equation (2.6) and approximate $\partial x / \partial \tau$.

The implementation of the complex-step method using either the method of steps or the dde23 Matlab solver does not give the correct solution (see Figure 2).

As we can see from Figure 2, the complex-step approximate of $dx/d\tau$ and the corresponding solution of the sensitivity equation is accurate only from the left side at $t = 0.5$.

EXAMPLE 2. In this example we consider a delay system where the history function is a step function with ten jump discontinuities and with the property that $d\phi/d\theta = 0, \ \theta \in$



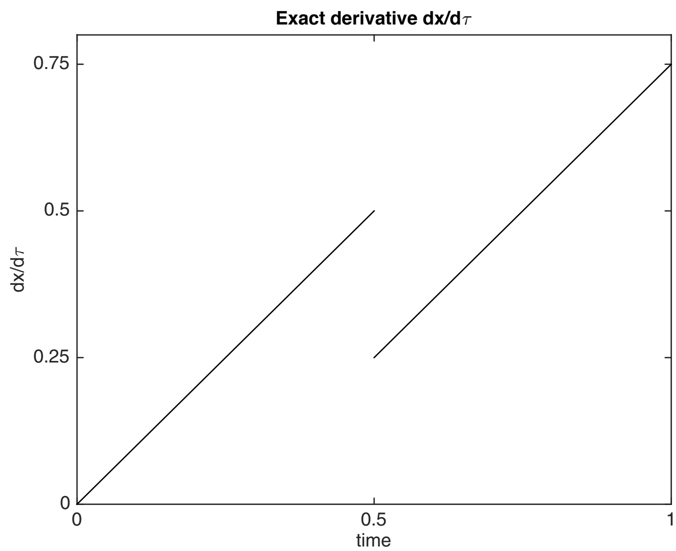


FIG. 2. Complex-step approximation of $dx/d\tau$ (top) and exact derivative $dx/d\tau$ (bottom) of the solution of DDEs in Example 1 for $\tau = 1$.

$(-\tau, 0)$, producing a continuous but not continuously differentiable solution $x(t)$.

$$\frac{dx}{dt}(t) = x(t-\tau;\tau),\ t \in (0,1], \tag{3.7}$$

$$x(\theta) = \phi(\theta) = \begin{cases} 0, & \theta \in \left[\frac{-2n\tau}{10}, \frac{-(2n-1)\tau}{10}\right),\ n = 1,\dots,5, \\ 1, & \theta \in \left[\frac{-(2n-1)\tau}{10}, \frac{-(2n-2)\tau}{10}\right), n = 2,\dots,5, \\ 1, & \theta \in [-\frac{\tau}{10}, 0]. \end{cases} \tag{3.8}$$

The exact solution for this system is given by

$$x(t) = \begin{cases} 1 + \frac{n}{10}\tau, & t \in \left[\frac{(2n)\tau}{10}, \frac{(2n+1)\tau}{10}\right],\ n = 0, \dots, 4, \\ 1 - \frac{n}{10}\tau + t, & t \in \left[\frac{(2n-1)\tau}{10}, \frac{(2n)\tau}{10}\right], n = 1, \dots, 5. \end{cases} \tag{3.9}$$

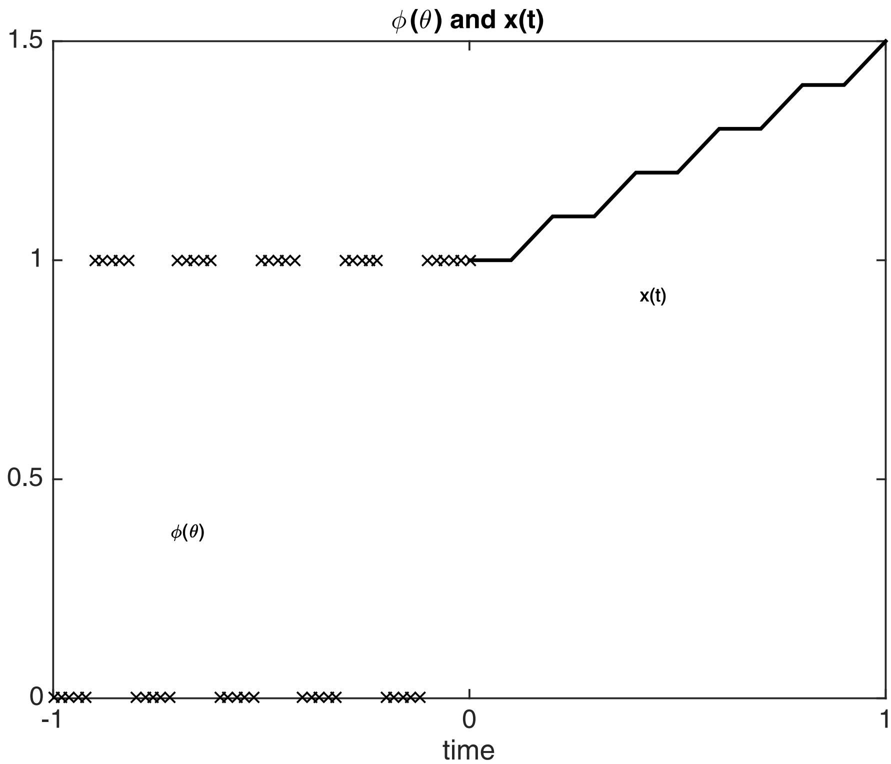


FIG. 3. Solution and history functions of Example 2 for $\tau = 1$.

The exact derivative is given by

$$\frac{\partial x}{\partial \tau}(t) = \begin{cases} \frac{n}{10}, & t \in \left(\frac{(2n)\tau}{10}, \frac{(2n+1)\tau}{10}\right),\ n = 0, \dots, 4, \\ -\frac{n}{10}, & t \in \left(\frac{(2n-1)\tau}{10}, \frac{(2n)\tau}{10}\right),\ n = 1, \dots, 5. \end{cases} \tag{3.10}$$

We implement the complex-step method to approximate $dx/d\tau$ as explained in Example 1 with the given step size $h = 10^{-40}$.

Here as we can see from Figure 4 (top), the complex-step does not approximate $dx/d\tau$ accurately due to the fact the jumps in the initial data results in subsequent jumps in the solution derivatives (i.e., corners in $x(t)$) later in time.

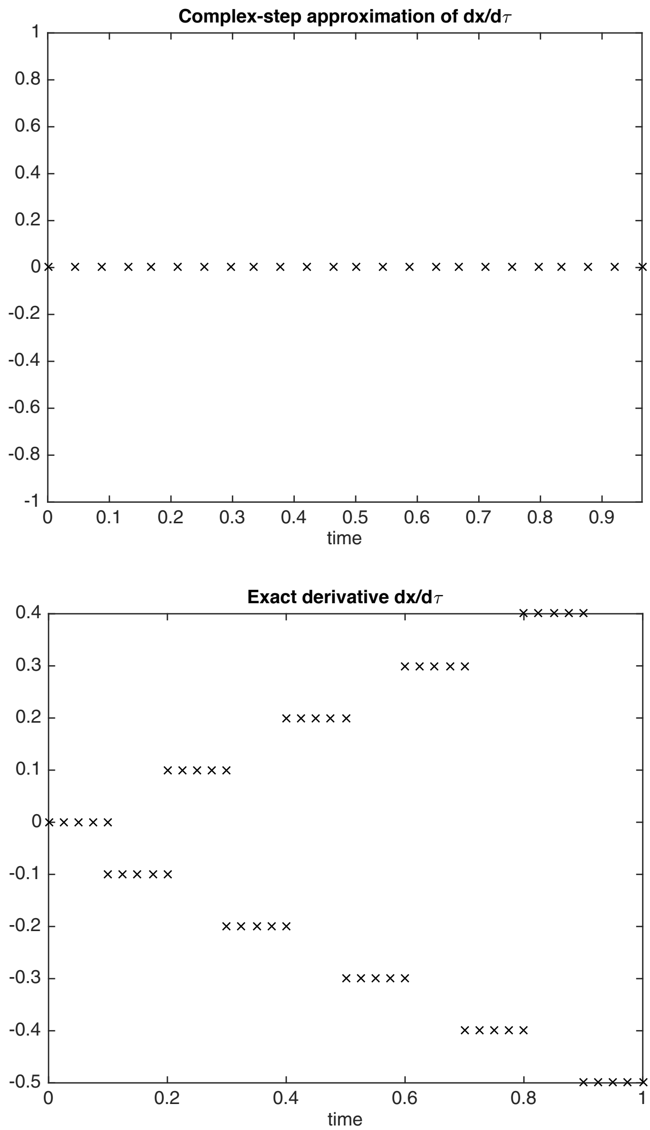


Fig. 4. Complex-step approximation of $dx/d\tau$ (top) and exact derivative $dx/d\tau$ (bottom) of the solution of DDEs in Example 2 for $\tau = 1$.

Example 3. In this third example, we consider a system of DDEs where the history function has one removable discontinuity producing a solution with matching right and left hand side derivatives.

$$\frac{dx}{dt}(t) = x(t-\tau;\tau),\ t \in (0,T], \tag{3.11}$$

$$x(\theta) = \phi(\theta) = \begin{cases} 3/4, & \theta = -\tau/2, \\ -\theta, & \theta \in [-\tau, -\tau/2) \cup (-\tau/2, 0]. \end{cases} \tag{3.12}$$

The exact solution for this problem is given almost everywhere by

$$x(t) = -t^2/2 + \tau t, \quad t \in [0,\tau],$$

and the exact derivative is given by

$$\frac{dx}{d\tau}(t) = \begin{cases} 0, & t = \tau/2, \\ t, & t \in [0,\tau/2) \cup (\tau/2,\tau). \end{cases}$$

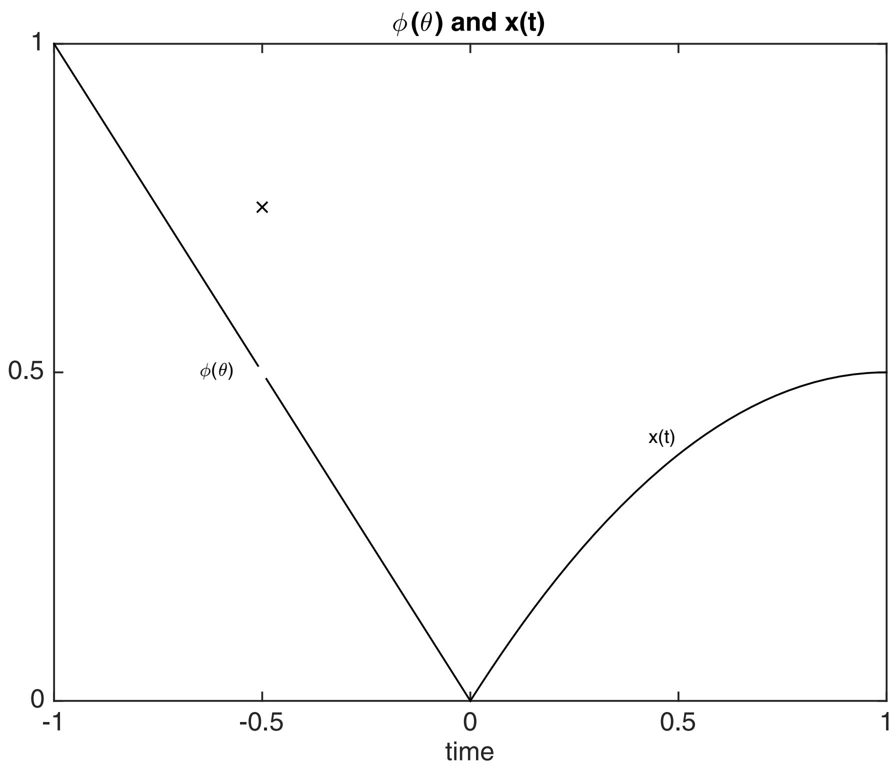


FIG. 5. Solution and history functions of Example 2 for $\tau = 1$.

Again, letting $s(t) = \frac{\partial x(t)}{\partial \tau}$, we have the sensitivity system:

$$\begin{aligned} \frac{ds}{dt}(t) &= -\dot{x}(t-\tau) + s(t-\tau),\ t > 0, \\ s(\theta) &= 0, \quad -\tau \le \theta \le 0, \end{aligned}$$

where

$$\dot{x}(t-\tau) = \begin{cases} -1 & \text{for} \quad 0 \le t < \tau/2, \\ -1 & \text{for} \quad \tau/2 < t \le \tau. \end{cases}$$

Again, this system is not well defined because $s(\tau/2)$ or $\dot{x}(-\tau/2)$ has no value.

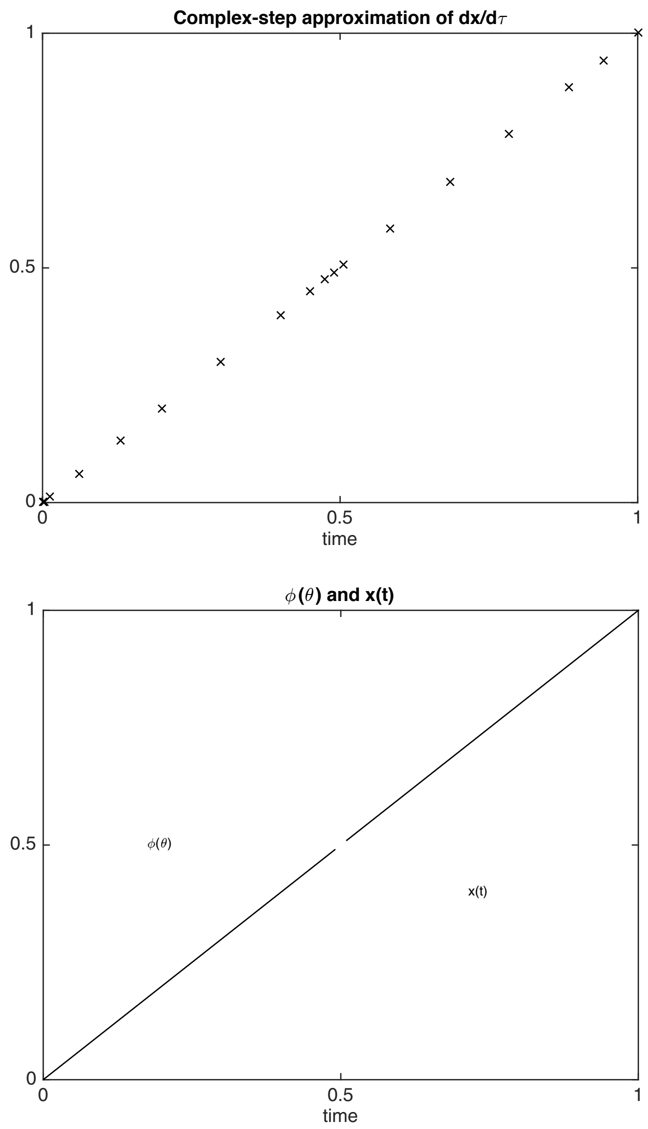


FIG. 6. Complex-step approximation of $dx/d\tau$ (top) and exact derivative $dx/d\tau$ (bottom) of the solution of DDEs in Example 3 for $\tau = 1$.

From Figure 6, we see that the complex-step method approximation of $\frac{dx}{d\tau}$ is accurate except at $t = \frac{\tau}{2}$. This is because

$$\lim_{h\to 0^-} \frac{\mathrm{Im}[x(\tau/2;\tau/2+ih)]}{h} = \lim_{h\to 0^+} \frac{\mathrm{Im}[x(\tau/2;\tau/2+ih)]}{h},$$

even though $s(\tau/2) = s(1/2)$ is not defined.

Example 4. In this last example we consider a DDE system with distribution history 'function'. Here not only the history function lacks smoothness (it is in $H^{-1}[-\tau, 0]$), but the solution function $x(t)$ has a jump at $t = \tau/2$.

$$\frac{dx}{dt}(t) = x(t-\tau;\tau), \quad t \in (0, T], \tag{3.13}$$

$$x(\theta) = \phi(\theta) = \delta(\theta + \tau/2), \quad \theta \in [-\tau, 0]. \tag{3.14}$$

The exact solution to this system is given on $[0, \tau]$ by

$$x(t) = \frac{d}{dt}\max\{t, \frac{\tau}{2}\}. \tag{3.15}$$

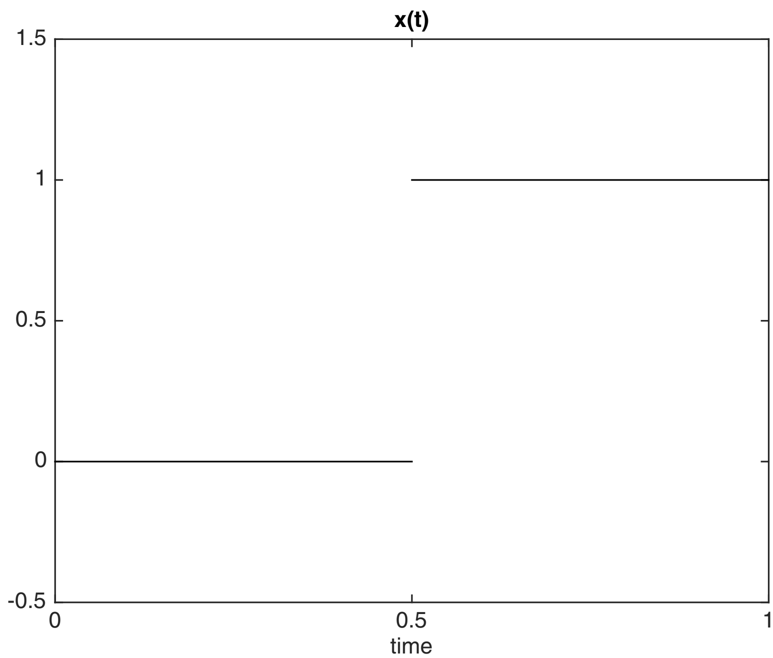


Fig. 7. Solution function of Example 4 for $\tau = 1$.

Before computing $dx/d\tau$ numerically, we define the Dirac-delta distribution as a limit as follows:
Consider a function b defined by

$$b(\xi;\epsilon) = \begin{cases} 0 & \text{if } |\xi + \tau/2| > \epsilon/2, \\ 1/\epsilon & \text{if } |\xi + \tau/2| < \epsilon/2. \end{cases} \tag{3.16}$$

Then, the history function takes the form

$$\phi(\xi) = \delta(\xi + \tau/2) = \lim_{\epsilon \to 0} b(\xi; \epsilon),$$

that is, for a very small ϵ,

$$\phi(\xi) = \delta(\xi + \tau/2) \approx b(\xi; \epsilon),$$

and for our computation, we take $\epsilon = 1 \cdot 10^{-10}$.

We compute $dx/d\tau$ using the complex-step method for $t \in [0, 1]$ and $\tau = 1$.

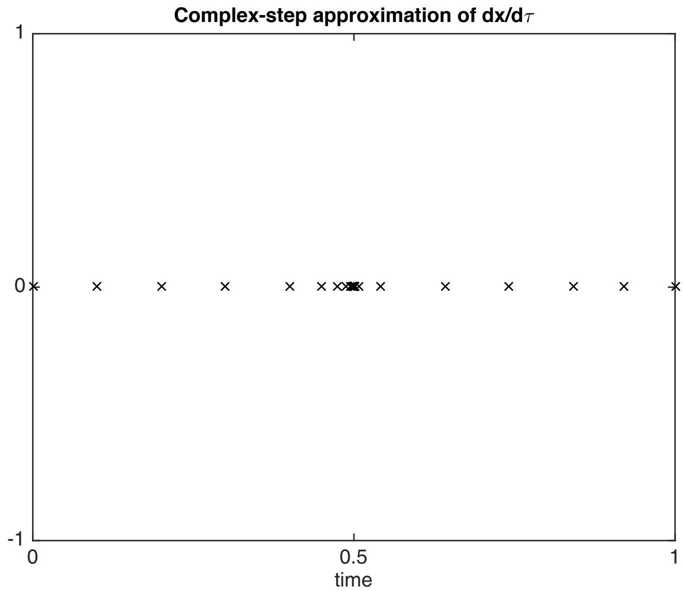


FIG. 8. Complex-step approximation of $dx/d\tau$ of the solution of DDEs in Example 4 for $\tau = 1$.

Here we see that even though $dx/d\tau$ is not defined at $t = \tau/2$, the complex-step implementation provides an accurate approximation of $dx/d\tau$ up to $t = \tau/2$ (see Figure 8). This is due to the fact that

$$\lim_{h \to 0^-} \frac{\mathrm{Im}[x(\cdot; \tau/2 + ih)]}{h} = \lim_{h \to 0^+} \frac{\mathrm{Im}[x(\cdot; \tau/2 + ih)]}{h} = 0.$$

4. Conclusions and further remarks. We applied the complex-step method to compute sensitivities for delay differential equations with various degree of discontinuities. Our findings show that discontinuities affect the accuracy of the complex-step approximation of the sensitivity when the discontinuities in the history result in corners or jumps in the solution for $t > 0$. Regardless of the non-smoothness of the initial data, the complex-step implementation using the method of steps and the Matlab solver dde23 provides accurate approximation of the *one-sided derivatives when they exist and are equal.* But we caution especially against the use of dde23 for delay equations with non-smoothness in the initial data. Our computations revealed that cavalier use of dde23 and the complex-step method in this case often produce incorrect results without any warning that the results are in error. In particular see Example 1, Figure 2, where the complex-step method and the dde23 solution of the sensitivity equation for $\frac{dx}{d\tau}$ produced incorrect results.

Having observed features of the behavior of the compelx-step method in delay equations, we turned next to a simple ordinary differential in attempts to further understand the complex-step method in the context of simpler systems of the form (1.1) and in particular the simple scalar equation $\frac{dx}{dt} = g(t, x; a) = -f(a)x(t)$ where the parameter a ranges over the values $(0, 1)$ and the function $f(a)$ is the quadratic a^2. If we consider $\frac{dx}{da}$ at $a = 1/2$ the complex-step method returns

$$\frac{dx}{da}(\xi; 1/2) = \lim_{h\to 0^-} \frac{\mathrm{Im}[x(\xi, 1/2 + ih)]}{h} = \lim_{h\to 0^+} \frac{\mathrm{Im}[x(\xi, 1/2 + ih)]}{h} = -2(1/2)\xi e^{-(1/2)^2\xi}.$$

In fact this yields the correct results and one can argue this since we have that for any C^2 function in q, the 2nd order Taylor expansion

$$x(t; q + ih) = x(t; q) + ih\frac{\partial x}{\partial q}(t; q) + \mathcal{R}_2(h)$$

where

$$\lim \frac{\mathcal{R}_2(h)}{h} = 0.$$

If we next consider the example with the same function $f(a)$ except at $a = 1/2$ where f takes on the value $f(1/2) = 1/2$, we find the limits

$$\lim_{h\to 0^-} \frac{\mathrm{Im}[x(\xi; 1/2 + ih)]}{h} = \lim_{h\to 0^+} \frac{\mathrm{Im}[x(\xi; 1/2 + ih)]}{h} = -2(1/2)\xi e^{-(1/2)^2\xi}$$

which are the same results even though $\frac{dx}{da}$ at $a = 1/2$ *does not exist.* The corresponding graphs are depicted in Example 5 below which reveal the strengths and weaknesses of using a complex expansion approach to finding sensitivity functions.

Example 5 (A simple ordinary differential equation). We seek a function $x(t)$ such that

$$\dot{x} = -f(a)x(t), \quad a.e. t > 0, \tag{4.1}$$

$$x(0) = 1, \tag{4.2}$$

where

$$f(a) = \begin{cases} a^2, & a \neq 1/2, \\ 1/2, & a = 1/2. \end{cases}$$

The solution is given by

$$x(t; a) = e^{-a^2 t} \tag{4.3}$$

so that

$$\dot{x} = -f(a)x(t)$$

almost everywhere in $t > 0$, and the exact derivative dx/da is given by

$$\frac{dx}{da}(t; a) = (-2at)e^{-a^2 t}, \quad a \neq 1/2. \tag{4.4}$$

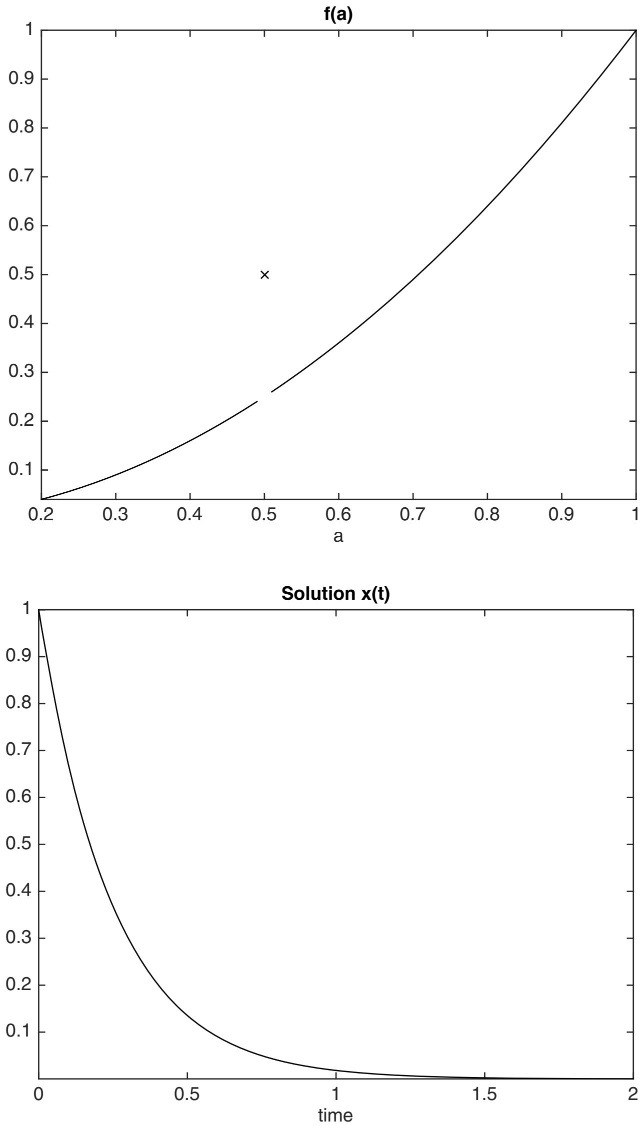


FIG. 9. Right hand side data $f(a)$ (top) and solution $x(t;2)$ of the ODE in Example 5 (bottom).

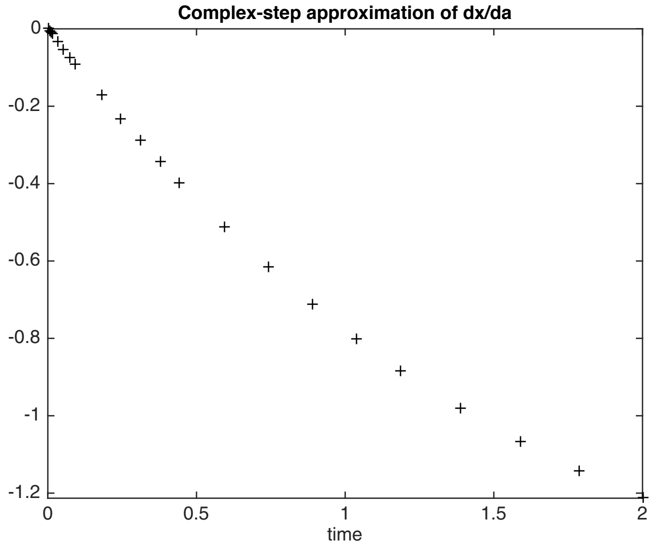


FIG. 10. Complex-step derivative approximation of dx/da for example 5 for $a = 1/2$ (Note that dx/da does not exist at $a = 1/2$.)

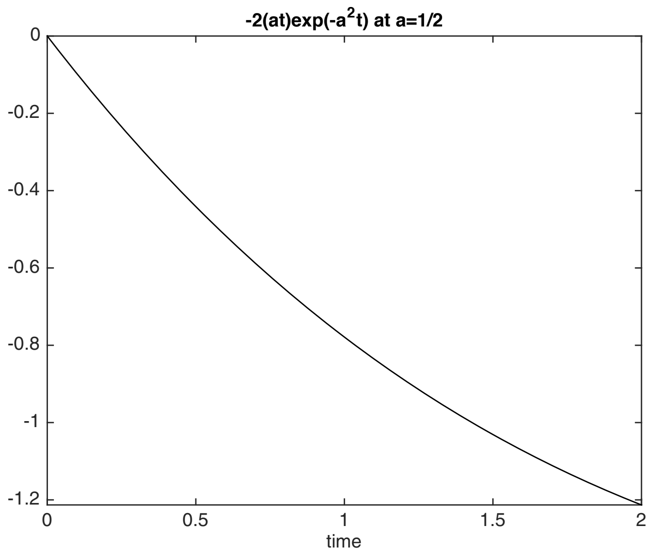


FIG. 11. $(-2at)e^{-a^2t}$ at $a = 1/2$.

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