Pitfalls in Parameter Estimation for Delay Differential Equations

C.T.H. Baker and C.A.H. Paul

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Pitfalls in Parameter Estimation for Delay Differential Equations

Christopher T.H. Baker* and Christopher A.H. Paul*

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In honour of Bill Gear on the celebration of his sixtieth birthday.

Abstract

Given a set of data \( \{ U(\gamma_i) \approx u(\gamma_i; p^*) \} \) corresponding to the delay differential equation

\[
\begin{align*}
    u'(t; p) &= f(t, u(t; p), u(\alpha(t; p); p); p) \text{ for } t \geq t_0(p), \\
    u(t; p) &= \Psi(t; p) \text{ for } t \leq t_0(p),
\end{align*}
\]

the basic problem addressed here is that of calculating the vector \( p^* \in \mathbb{R}^n \). (We also consider neutral differential equations.) Most approaches to parameter estimation calculate \( p^* \) by minimizing a suitable objective function that is assumed to be sufficiently smooth. In this paper, we use the derivative discontinuity tracking theory for delay differential equations to analyze how jumps can arise in the derivatives of a natural objective function. These jumps can occur when estimating parameters in lag functions and estimating the position of the initial point, and as such are not expected to occur in parameter estimation problems for ordinary differential equations.

Key words.  Parameter estimation, delay differential equations, derivative discontinuities.

AMS subject classifications.  65K10, 65Q05

* Mathematics Department, University of Manchester, Manchester M13 9PL, ENGLAND.
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1 Introduction

The typical parameter estimation problem may be summarized as, “Given values of a solution, what was the problem?”. The problem of estimating unknown parameters in functional equations, in particular delay differential equations (DDEs), has been brought to our attention in the context of modelling cell proliferation phenomena (see [2, 6], for example). For the numerical solution of DDEs and for parameter estimation in ordinary differential equations (ODEs), we refer to [1] and [10] and their references, respectively. A parameter estimation problem may be resolved by minimizing a suitable objective function. The principal message in this paper is that this objective function may not be sufficiently smooth, an observation that has practical consequences in the optimization process.

1.1 The Problem

Given the parameterized state-independent DDE

\[
\begin{align*}
  u'(t; p) &= f(t, u(t; p), u(\alpha(t; p); p); p) \quad (t \geq t_0(p)), \\
  u(t; p) &= \Psi(t; p) \quad (t \leq t_0(p)),
\end{align*}
\]

(1)

where \( p \in \mathbb{R}^n \) and \( \alpha(t; p) \) is continuous, and solution values \( \{U(\gamma_i) \approx u(\gamma_i; p^*)\} \), the parameter estimation problem is that of estimating the vector \( p^* \). This is generally achieved by minimizing an objective function involving the data \( \{U(\gamma_i)\} \) and the corresponding values of the parameterized solution \( \{u(\gamma_i; p)\} \) over \( p \). We assume that (1) is smoothly dependent on \( p \). Later our discussion will include more general forms of (1), including state-dependent DDEs, and neutral differential equations (NDEs) (where \( u'(t; p) \) also depends on derivatives evaluated at delayed arguments). If \( \alpha(t; p) > t \) then (1) becomes an advanced differential equation (ADE), which requires different treatment from that for DDEs and NDEs. The occurrence of ADEs may be avoided by imposing the non-linear functional constraint \( \alpha(t; p) \leq t \) in the minimization process.

A common objective function is based on the squared two-norm (see [10]),

\[
\Phi(p) = \sum_i [U(\gamma_i) - u(\gamma_i; p)]^2,
\]

(2)

because it is generally continuous (and hopefully smooth) with respect to variations in \( p \). Throughout this paper we shall use (2) as our objective function. We shall produce examples that demonstrate that this objective function need not be smooth.

The problem of estimating the vector \( p^* \) that corresponds to the data \( \{U(\gamma_i)\} \) is solved by calculating some ‘best-fit’ parameter value \( p^\sharp \) that minimizes \( \Phi(p) \). In the idealized scenario, we may suppose that \( \{U(\gamma_i) \equiv u(\gamma_i; p^*)\} \) and one such value of \( p^\sharp \) is then \( p^* \). The precise nature of the values \( \{U(\gamma_i)\} \) has little effect on our discussion of smoothness,
except that there is some local smoothing of the objective function when \( u(\gamma_i; p) = U(\gamma_i) \), such as in the idealised scenario with \( p = p^* \).

### 1.2 Further Notation

The notation \( \varphi'(t) \) usually denotes the derivative \( d\varphi/dt \), and the implication is that the left- and right-hand derivatives

\[
\left( \frac{d\varphi(t)}{dt} \right)_- \equiv \varphi_-(t) = \lim_{\delta \searrow 0} \left[ \frac{\varphi(t) - \varphi(t - \delta)}{\delta} \right],
\]

\[
\left( \frac{d\varphi(t)}{dt} \right)_+ \equiv \varphi_+(t) = \lim_{\delta \nearrow 0} \left[ \frac{\varphi(t + \delta) - \varphi(t)}{\delta} \right]
\]

both exist and are equal. In addition, we shall write

\[
\varphi^{(s)}_\pm(t) := \left( \frac{d^{s-1}\varphi_\pm(t)}{dt^{s-1}} \right) \quad \text{for } s = 1, 2, \ldots \quad (\varphi^{(0)}_\pm(t) = \varphi(t)).
\]

We say that “the derivative \( \varphi^{(r)}(t) \) has a jump\(^1\) at \( t = s \) when the left- and right-hand derivatives both exist at \( t = s \) and \( 0 < |\varphi^{(r)}_+(s) - \varphi^{(r)}_-(s)| < \infty \)”. If, for some \( \delta > 0 \), \( \varphi^{(r)}_+(t) \) exists for \( t \in [s - \delta, s) \) and \( t \in [s, s + \delta] \), then \( \varphi^{(r)}(t) \) has a jump at \( t = s \) when \( \lim_{t\searrow s} \varphi^{(r)}_+(t) \neq \varphi^{(r)}_-(s) \). A function \( \varphi(t) \) is said to be smoother than a function \( \psi(t) \) at \( t = s \) if \( \varphi^{(r)}(s) \) exists but \( \psi^{(r)}(s) \) does not exist. Similar notation and terminology applies to the partial derivatives of functions of more than one variable.

Due to the existence of discontinuities in \( u(t; p) \), all derivatives of \( u(t; p) \) with respect to \( t \) are taken to be the right-hand derivatives, so that (1) is interpreted as

\[
u'_+(t; p) = f(t, u(t; p), u(\alpha(t; p); p); p) \quad (t \geq t_0(p)); \quad u(t, p) = \Psi(t; p) \quad (t \leq t_0(p)).
\]

By a discontinuity, we mean a jump in \( u(t; p) \) or one of its derivatives.

### 1.3 Organisation of the paper

We establish in Section 2 that the objective function can be non-smooth due to discontinuities in the solution of (1). We also show that it may be smooth despite such discontinuities. Our conclusions are illustrated in Section 3 with some graphs of computed partial derivatives of \( \Phi(p) \) for the following parameter estimation problems:

\[
\begin{align*}
u'(t) &= \lambda u(t - 1) \quad (t \geq 0), \quad u(t) = 1 \quad (t \leq 0), \quad p = [\lambda]; \\
u'(t) &= \lambda u(\nu t) \quad (t \geq 1), \quad u(t) = 2 \quad (t < 1), \quad u(1) = 0, \quad p = [\lambda, \nu]; \\
u'(t) &= \lambda u(\tau - t) \quad (t \geq 0), \quad u(t) = \beta \cos(t) \quad (t \leq 0), \quad p = [\lambda, \tau, \beta]; \\
u'(t) &= \lambda u(t) + \nu u(u(t) - 1) \quad (t \geq 0), \quad u(t) = \beta \cos(t) \quad (t \leq 0), \quad p = [\lambda, \nu, \beta]; \\
u'(t) &= \lambda u(t - 1) \quad (t \geq t_0), \quad u(t) = \cos(t) \quad (t < t_0), \quad u(t_0) = 0, \quad p = [\lambda, t_0].
\end{align*}
\]

\(^1\)For convenience we only consider finite jumps.
2 The Objective Function and its Derivatives

We first recall some properties of the solutions of DDEs, and then indicate the consequences for the smoothness of the objective function (2).

2.1 Propagation of Discontinuities in DDEs

It is well-known [8, 9] that discontinuities can arise and propagate in the solutions of DDEs and NDEs. For example, in the case of the constant lag DDE

\[ u'(t) = \lambda u(t - \tau) \quad \text{for} \quad t \geq t_0, \quad u(t) = 1 \quad \text{for} \quad t \leq t_0, \]

a jump occurs in \( u'(t) \) at \( t = t_0 \) if \( \lambda \neq 0 \), since \( u'_-(t_0) = 0 \) and \( u'_+(t_0) = \lambda u(-\tau) = \lambda \).

Simple analysis shows that this jump propagates to the points \( t = t_0 + \tau, t_0 + 2\tau, \ldots \). In fact \( u^{(n+1)}_\pm(t) = \lambda^n u'_\pm(t - n\tau) \), so that a jump in \( u'(t) \) at \( t = t_0 \) \( u'_-(t_0) \neq u'_+(t_0) \) propagates to one in \( u''(t) \) at \( t = t_0 + \tau \) \( u''_-(t_0 + \tau) \neq u''_+(t_0 + \tau) \) and then to one in \( u'''(t) \) at \( t = t_0 + 2\tau \), hence \( u(t) \) becomes smoother as \( t \) increases. This smoothing is typical of a DDE in which \( \alpha(t) \) is monotonic increasing. A similar analysis shows that discontinuities in NDEs are not usually smoothed: For example, for the equation

\[ u'(t) = \lambda u'(t - \tau) \quad \text{for} \quad t \geq t_0, \quad u(t) = \Psi(t) \quad \text{for} \quad t \leq t_0, \]

we have that \( u'_-(t_0) = \Psi'(t_0) \) and \( u'_+(t_0) = \lambda \Psi'(t_0 - \tau) \), and these values need not agree. Now \( u'_+(t) = \lambda^n u'_+(t - n\tau) \), so that \( u'_+(t_0 + n\tau) = \lambda^n u'_+(t_0) \). Thus \( u(t) \) does not become smoother as \( t \) increases and the size of the jump in \( u'(t) \) is magnified by a factor \( \lambda \) each time that it propagates.

For both DDEs and NDEs, assuming that \( f \) is smooth, a discontinuity only propagates to a point \( \sigma_k \), say, when a previous discontinuity point \( \sigma_j \) is crossed by the delayed argument \( \alpha(t) \) at \( t = \sigma_k \). That is to say, there exists a finite \( \delta > 0 \) such that \( [\alpha(\sigma_k + \delta) - \sigma_j][\alpha(\sigma_k - \delta) - \sigma_j] < 0 \).

2.2 Consequences for Parameter Estimation

We have indicated how a discontinuity can arise and propagate in the solution of a DDE and an NDE. We suppose that jumps in the derivatives of \( u(t; p) \) with respect to \( t \) occur at the points

\[ \Sigma(p) \equiv \{ \sigma_1(p), \sigma_2(p), \ldots \}. \]

Such discontinuities, when arising from the initial point \( t_0(p) \) (and the initial function \( \Psi(t; p) \)), may propagate into \( \Phi(p) \) via the solution values \( \{ u(\gamma_i; p) \} \). We shall now investigate in what circumstances this can occur.

\(^2\)Discontinuity propagation in scalar DDEs is discussed in [8]; also see [9].
Theorem 2.1 We have the results

\[
\left( \frac{\partial \Phi(\gamma_i; p)}{\partial p_t} \right)_\pm = -2 \sum_i [U(\gamma_i) - u(\gamma_i; p)] \left( \frac{\partial u(\gamma_i; p)}{\partial p_t} \right)_\pm,
\]

\[
\left( \frac{\partial^2 \Phi(\gamma_i; p)}{\partial p_t \partial p_m} \right)_\pm = 2 \sum_i \left[ \left( \frac{\partial u(\gamma_i; p)}{\partial p_t} \right)_\pm \left( \frac{\partial u(\gamma_i; p)}{\partial p_m} \right)_\pm - [U(\gamma_i) - u(\gamma_i; p)] \left( \frac{\partial^2 u(\gamma_i; p)}{\partial p_t \partial p_m} \right)_\pm \right].
\]

Proof. By elementary differentiation of (2).

It is clear from Theorem 2.1 that a jump in a first partial derivative of \( \Phi(p) \) can occur if

\[
u_\ell(t; p) := \frac{\partial u(t; p)}{\partial p_\ell}
\]

has a jump at \( t = \gamma_i \) for at least one \( i \). However, the jump does not propagate into \( \partial \Phi / \partial p_\ell \) if \( U(\gamma_i) = u(\gamma_i; p) \), in particular if \( p = p^* \) in the idealized scenario. (Also, if jumps occur in \( u_\ell(t; p) \) at more than one \( \gamma_i \), then there is a possibility that they may cancel each other out.) Sufficient insight on jumps in the second partial derivatives of \( \Phi(p) \) is obtained if we restrict our attention to the case that \( m = \ell \). A jump in

\[w_\ell(t; p) := \frac{\partial^2 u(t; p)}{\partial p^2_\ell}\]

at \( t = \gamma_i \) can propagate into \( \partial^2 \Phi / \partial p^2_\ell \), but will not do so if \( U(\gamma_i) = u(\gamma_i; p) \) (again, in particular if \( p = p^* \) in the idealized scenario).

By Theorem 2.1, jumps in the partial derivatives of \( \Phi(p) \) can arise from corresponding jumps in the partial derivatives of \( u(t; p) \). To establish the connection between jumps in the derivatives of \( u(t; p) \) with respect to \( t \) and those in \( \Phi(p) \) with respect to some \( p_\ell \), we return to equation (1). Here we regard \( t_0 \) as independent of \( p \), for convenience. We differentiate \( u'(t; p) \) with respect to \( p_\ell \) to obtain a system of two coupled equations, but first we introduce the following notation:

\[
\begin{align*}
f_x(t, x, y; p) &= \frac{\partial}{\partial x} f(t, x, y; p), & f_\ell(t, x, y; p) &= \frac{\partial}{\partial p_\ell} f(t, x, y; p), & \alpha_\ell(t; p) &= \frac{\partial}{\partial p_\ell} \alpha(t; p), \\
f_y(t, x, y; p) &= \frac{\partial}{\partial y} f(t, x, y; p), & \Psi_\ell(t; p) &= \frac{\partial}{\partial p_\ell} \Psi(t; p).
\end{align*}
\]

Theorem 2.2 Formally, for a state-independent DDE, we have

\[
\begin{align*}
u'(t; p) &= f(t, u(t; p), u(\alpha(t; p); p); p) \\
u_\ell'(t; p) &= f_x(t, u(t; p), u(\alpha(t; p); p); p) \times u_\ell(t; p) + f_y(t, u(t; p), u(\alpha(t; p); p); p) \times \alpha_\ell(t; p) \times u_\ell(t; p) + f_\ell(t, u(t; p), u(\alpha(t; p); p); p) \\
u(t; p) &= \Psi(t; p) \\
u_\ell(t; p) &= \Psi_\ell(t; p)
\end{align*}
\]

(4) \( (t \geq t_0) \),

\( (t \leq t_0) \).
Proof. By elementary differentiation of (1).

In general the formal derivation of \( u'_\ell(t; p) \) is valid if \( t \not\in \Sigma(p) \). To investigate the behaviour of \( u_\ell(t; p) \) a further differentiation of \( u'_\ell(t; p) \) is required, producing a system of three coupled equations. Although equation (1) is a DDE, in general the system of equations (4) is a neutral system.

Assuming the validity of (4), the points at which jumps can occur in the derivatives of \( u_\ell(t; p) \) with respect to \( t \) can be obtained from (4); they are intimately related\(^3\) to the positions \( \Sigma(p) \) of the jumps in derivatives of \( u(t; p) \) with respect to \( t \). However, it is precisely at such points that (4) may not be justified. In general, therefore, we may expect \( u_\ell(t; p) \) to have a jump at the point \( t = s \) if \( s \in \Sigma(p) \). The complexity of the equations for \( u_\ell(t; p) \) does not allow easy insight into the propagation of discontinuities from \( u(t; p) \) into \( u_\ell(t; p) \), except in special cases. We shall adopt a different approach in order to establish a particular feature. At issue is the behaviour of \( u_\ell(t; p) \) and its derivatives with respect to the variables \( \{ p_j \} \). Let us suppose that the derivatives in (4) are all right-hand derivatives and that

\[
\lim_{t \to \sigma_r(p)} u_\ell(t; p) \neq u_\ell(\sigma_r(p); p) \text{ for some } r,
\]

then \( u_\ell(t; p) \) has a jump at the point \( \sigma_r(p) \in \Sigma(p) \). If \( u(\sigma_r(p); p) \) varies smoothly with respect to \( p_\ell \) when the other components of \( p \) are fixed, then \( du(\sigma_r(p); p)/dp_\ell \) has no jumps. Thus, since

\[
\frac{du(\sigma_r(p); p)}{dp_\ell} = u'(t; p)|_{t=\sigma_r(p)} \times \frac{\partial \sigma_r(p)}{\partial p_\ell} + u_\ell(t; p)|_{t=\sigma_r(p)},
\]

we see that if \( u'(t; p) \) has a jump at \( t = \sigma_r(p) \) and \( \partial \sigma_r(p)/\partial p_\ell \) does not vanish, then \( u_\ell(t; p) \) must also have a jump at \( t = \sigma_r(p) \). It follows that \( \partial u(\gamma_i; p)/\partial p_\ell \) has a jump provided that \( \gamma_i = \sigma_r(p) \) for some \( r \) and \( \sigma_r(p) \) varies as \( p_\ell \) varies.

We shall illustrate the types of argument used above by reference to particular examples.

3 Numerical Examples

In this section we present, in graphical form, evidence that supports the various conclusions summarized in our closing section. In cases where the partial derivatives of \( \Phi(p) \) are smooth, graphical evidence is not presented.

Example 3.1 We commence with the problem of determining \( \lambda \) in the DDE

\[
u'(t; p) = \lambda u(t-1; p) \text{ for } t \geq 0, \quad u(t; p) = 1 \text{ for } t \leq 0,
\]

\(^3\)Similar network dependencies to those in [9] apply but, typically, there is no smoothing.
where \( p = [\lambda] \). The set \( \{U(\gamma_i)\} \) consists of values of the solution for some \( \lambda = \lambda^* \neq 0 \). Although \( u^{(r)}(t) \) has a jump at \( t = r - 1 \), the objective function \( \Phi(p) \) is smooth for any choice of \( \{\gamma_i\} \). In fact

\[
u(t; p) = \sum_{n=0}^{[t]+1} \frac{\lambda^n(t - n + 1)^n}{n!},
\]

where \([z]\) denotes the integer part of \( z \); this permits an explicit expression for \( \Phi(p) \). Furthermore, if \( u_\lambda(t; p) = \partial u(t; p)/\partial \lambda \), then

\[
u_\lambda(t; p) = \lambda u_\lambda(t - 1; p) + u(t - 1; p) \quad \text{for} \quad t \in (0, 1) \cup (1, \infty), \quad u_\lambda(t; p) = 0 \quad \text{for} \quad t \leq 0.
\]

The latter equation holds for all \( t \geq 0 \) when the derivative with respect to \( t \) is taken as the right-hand derivative. The explicit form of \( u_\lambda(t; p) \) can be obtained from (5),

\[
u_\lambda(t; p) = \sum_{n=1}^{[t]+1} \frac{\lambda^n-1(t - n + 1)^n}{(n-1)!}.
\]

Note that \( u_\lambda(t; p) \) is continuous for \( t \geq 0 \), and hence \( \partial \Phi/\partial \lambda \) has no jumps.

\[\diamond\]

**Example 3.2** We consider

\[
u'(t; p) = \lambda u(\nu t; p) \quad \text{for} \quad t \geq 1, \quad u(t; p) = 2 \quad \text{for} \quad t < 1, \quad u(1; p) = 0,
\]

where \( p = [\lambda, \nu] \). This is a DDE only if \( \nu \leq 1 \), since \( \alpha(t; p) = (1 - \nu)t \) must remain non-negative for all \( t \geq 1 \). The data \( \{U(\frac{3}{2}), U(\frac{1}{2}), U(\frac{5}{2}), U(\frac{7}{2}), U(\frac{9}{2})\} \) is obtained from (6) using \( p^* = [\frac{3}{2}, \frac{1}{2}] \). Simple analysis shows that jumps occur in \( u'(t; p) \) at \( t = 1/\nu \) and in \( u''(t; p) \) at \( t = 1/\nu^2 \), etc. For the function \( u_\nu(t; p) = \partial u(t; p)/\partial \nu \), we find that

\[
u_\nu(t; p) = \lambda t u'(\nu t; p) = \lambda^2 t u(\nu^2 t; p) \quad \text{for} \quad t \in (1, \frac{1}{\nu}) \cup (\frac{1}{\nu}, \infty), \quad u_\nu(t; p) = 0 \quad \text{for} \quad t \leq 1
\]

and for the function \( w_\nu(t; p) = \partial^2 u(t; p)/\partial \nu^2 \), we find that

\[
u_\nu(t; p) = 2 \nu \lambda^2 t^2 u'(\nu^2 t; p) \quad \text{for} \quad t \in (1, \frac{1}{\nu}) \cup (\frac{1}{\nu}, \frac{1}{\nu^2}) \cup (\frac{1}{\nu^2}, \infty), \quad w_\nu(t; p) = 0 \quad \text{for} \quad t \leq 1.
\]

Indeed, \( \partial/\partial \nu \) at \( u_\nu(t; p) \) for \( t \in (1, \frac{1}{\nu}) \cup (\frac{1}{\nu}, \infty) \), so that any jump in \( u_\nu(t; p) \) must occur at the point \( t = \frac{1}{\nu} \) and any additional jump in \( w_\nu(t; p) \) must occur at \( t = \frac{1}{\nu^2} \).

It follows from this that a jump may occur in \( \partial \Phi/\partial \nu \) when \( \nu = 1/\gamma_i \) for any \( i \); that is to say, when \( \nu \in \{\frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \frac{4}{5}, \frac{5}{6}, \frac{6}{7}, \frac{7}{8}\} \). Putting \( \lambda = \frac{3}{4} \) ensures that there is no smoothing of the discontinuity in \( u_\nu(t; p) \) as it propagates into \( \partial \Phi/\partial \nu \) at \( \nu = \frac{1}{2} \), and such jumps are clearly visible in Figure 1. The jumps in \( \partial^2 \Phi/\partial \nu^2 \) that occur at \( \nu \sqrt{1/\gamma_i} \) can also be deduced.

\[\diamond\]
The preceding examples are of DDEs with state-independent delays. In the remainder of this section we shall widen the class of equations to consider NDEs, DDEs with state-dependent delays, and DDEs in which the position of \( t_0 \) is parameter-dependent.

**Example 3.3** This example illustrates that, although the solution of an NDE may have many jumps in its first derivative, they can only propagate into \( \Phi(p) \) if a lag function is parameter-dependent. That is to say, the positions of the discontinuities in \( u(t; p) \) cross datapoints \( \{ \gamma_i \} \) as \( p \) varies, so that \( \partial \sigma(p)/\partial p_\ell \neq 0 \) for some \( p_\ell \). Consider

\[
u'(t; p) = \lambda u'(t - \tau; p) \quad \text{for} \quad t \geq 0, \quad u(t; p) = \beta \cos(t) \quad \text{for} \quad t \leq 0, \tag{7}\]

where \( p = [\lambda, \tau, \beta] \). The data \( \{ U(1/2), U(1), U(3/2), U(2), U(5/2), U(3) \} \) is obtained from (7) using \( p^* = [1, 1, 1] \), so that \( u'(t; p) \) has jumps at the points \( t = N \). However, no jumps occur in the partial derivatives of \( \Phi(p) \) with respect to either \( \lambda \) or \( \beta \). If the lag \( \tau \) is to be estimated, then the jumps in \( u'(t; p) \) occur at \( t = \tau N \). Thus \( \partial \Phi/\partial \tau \) may have jumps at \( \tau = \gamma_i/N \) for any \( i \).

![Figure 1: Jumps in \( \partial \Phi/\partial \nu \) for a DDE when \( \Psi(t_0; p) \neq u(t_0; p) \).](image1.png)

![Figure 2: Jumps in \( \partial \Phi/\partial \tau \) for an NDE when \( \Psi'(t_0; p) \neq u'(t_0; p) \).](image2.png)
Figure 2 shows that jumps occur in $\partial \Phi / \partial \tau$ at $\tau = \frac{3}{5}, \frac{5}{8}, \frac{2}{3}, \frac{5}{6}, \frac{5}{4}$ and in $\partial^2 \Phi / \partial \tau^2$ at $\tau = 1$. The occurrence and position of these jumps is exactly as predicted; in particular the smoothing of the discontinuity in $u_\tau(t; p)$ at $\tau = 3.5, 5.8, 2.3, 3.4, 5.6, 5.4$ and in $\partial^2 \Phi / \partial \tau^2$ at $\tau = 1$. The occurrence and position of these jumps is exactly as predicted; in particular the smoothing of the discontinuity in $u_\tau(t; p)$ at $\tau = 1$ (for which $U(t) \equiv u(t; p)$) as it propagates into $\Phi(p)$.

The next example is based on a state-dependent DDE so that, since the lag is dependent on the solution, jumps may occur in any of the partial derivatives of $\Phi(p)$.

Example 3.4 Consider

$$u'(t; p) = \lambda u(t; p) + \nu u(t; p) - 1; p)$$

for $t \geq 0$, $u(t; p) = \beta \cos(t)$ for $t \leq 0$, (8)

where $p = [\lambda, \nu, \beta]$. This problem gives a DDE only for certain values of the parameters – in particular $\beta \leq 1$, since $t + 1 - u(t; p)$ must be non-negative for $t \geq 0$. As the positions of the discontinuities in $u(t; p)$ depend on $u(t; p)$, it is difficult to predict a priori where jumps may arise in the partial derivatives of $\Phi(p)$. The data $\{U(1), U(2), U(3), U(4), U(5), U(6)\}$ is obtained from (8) using $p^* = [-1, -5, -\frac{1}{2}]$.

Figure 3: Jumps in $\partial \Phi / \partial \beta$ for a DDE when $\Psi'(t_0; p) \neq u'(t_0; p)$.

Figure 3 shows how the jump in $u'(t; p)$ at $t = t_0$ propagates into $\partial \Phi / \partial \beta$.

The final example shows how a jump can occur in $\Phi(p)$ itself:

Example 3.5 Consider estimating the position of the initial point $t_0(p)$ in the following DDE

$$u'(t; p) = \lambda u(t - 1; p) \quad \text{for} \quad t \geq t_0, \quad u(t; p) = \cos(t) \quad \text{for} \quad t < t_0, \quad u(t_0; p) = 0,$$

where $p = [\lambda, t_0]$. The data $\{U(\frac{-2}{3}), U(\frac{1}{3}), U(0), U(\frac{1}{4}), U(\frac{2}{7})\}$ is obtained from (9) using $p^* = [1, 0]$. Clearly $u(t; p)$ has a jump at $t = t_0$, except when $\cos(t_0) = 0$ in which case the jump occurs in $u'(t; p)$. Thus a jump may occur in $\Phi(p)$ when $t_0 = \gamma_i$ for any $i$, and these jumps can indeed be seen in Figure 4.
4 Conclusion

As a rule of thumb, the following conclusions may be formulated:

- A discontinuity can only occur in \( \Phi(p) \) when the position of a discontinuity in \( u(t; p) \) or in \( \Psi(t; p) \) crosses a datapoint \( \gamma_i \) as \( p \) varies.
- There is no smoothing of a discontinuity at \( t = \gamma_i \) as it propagates into \( \Phi(p) \), unless \( u(\gamma_i; p) = U(\gamma_i) \).

Assuming that there is no smoothing of a discontinuity as it propagates into \( \Phi(p) \):

- Jumps can arise in \( \Phi(p) \) when:
  1. \( \Psi(t_0; p) \neq u(t_0; p) \) and the initial point \( t_0(p) \) is being estimated.

- Jumps can arise in the first partial derivatives of \( \Phi(p) \) when:
  1. \( \Psi(t_0; p) \neq u(t_0; p) \) or \( \Psi(t; p) \) has a jump, or
  2. \( \Psi'(t_0; p) \neq u'(t_0; p) \) or \( \Psi'(t) \) has a jump, and (1) includes a neutral term, or
  3. \( \Psi'(t_0; p) \neq u'(t_0; p) \) and the initial point \( t_0(p) \) is being estimated.

- Jumps can arise in the second partial derivatives of \( \Phi(p) \) when:
  1. \( \Psi'(t_0; p) \neq u'(t_0; p) \) or \( \Psi'(t; p) \) has a jump, or
  2. \( \Psi''(t_0; p) \neq u''(t_0; p) \) or \( \Psi''(t; p) \) has a jump, and (1) includes a neutral term, or
  3. \( \Psi''(t_0; p) \neq u''(t_0; p) \) and the initial point \( t_0(p) \) is being estimated.
Final comments and Acknowledgements

The numerical analysis of parameter estimation in DDEs has previously been addressed in [3, 4, 5, 7]. Our work appears to be the first where the smoothness of the objective function has been investigated. The parameter estimation problem has been shown to be one where the objective function commonly used is not smooth; this can have practical implications when employing black-box optimization routines to locate a minimum $p^\star$.

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References


