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## Optimal control problems with delays in state and control and mixed control–state constraints

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## Abstract

Optimal control problems with delays in state and control variables are studied. Constraints are imposed as mixed control–state inequality constraints. Necessary optimality conditions in the form of Pontryagin’s minimum principle are established. The proof proceeds by augmenting the delayed control problem to a nondelayed problem with mixed terminal boundary conditions to which Pontryagin’s minimum principle is applicable. Discretization methods for the delayed control problem are discussed which amount to solving a large-scale nonlinear programming problem. It is shown that the Lagrange multipliers associated with the programming problem provide a consistent discretization of the advanced adjoint equation for the delayed control problem. An analytical example and two numerical examples from chemical engineering and economics illustrate the results.

## 1 Introduction

Differential control systems with delays in state or control variables play an important role in the modelling of real–life phenomena in various fields of applications. Many papers have been devoted to delayed (other terminology: time lag, retarded, hereditary) optimal control problems and the derivation of necessary optimality conditions. Let us briefly review some papers concerning different classes of control problems. An introduction to time delay control problems can be found in Oğuztöreli [24]. Kharatishvili [17] was first to provide a maximum principle for optimal control problems with a constant state delay. In [18], he gave similar results for control problems with pure control delays. Halany [14] proves a maximum principle for optimal control problems with multiple constant delays in state and control variables which, however, are chosen to be equal for state and control. Similar results were obtained by Ray, Soliman [30]. Guinn [13] sketches a simple method for obtaining necessary conditions for control problems with a constant delay in the state variable. He suggests to augment the delayed control problem which yields a higher-dimensional undelayed control problem to which the standard maximum principle is applicable. Banks [3] derives a maximum principle for control systems with a time-dependent delay in the state variable. Delays in the control are admitted for systems linear in the control variable. Colonius and Hinrichsen [8] provide a unified approach to control problems with delays in the state variable by applying the theory of necessary conditions for optimization problems in function spaces. All articles mentioned so far do not consider general control or state inequality constraints.

Angell and Kirsch [1] treat functional differential equations with function-space state inequality constraints. However, they do not discuss the regularity of the multiplier associated with the state constraint and do not provide a numerical example with a pure state space constraint. To our knowledge, optimal control problems with constant delays in state and control variables and *mixed control-state inequality constraints* have not yet

been considered in the literature. The first goal in this paper is to derive a Pontryagin type minimum (maximum) principle for this class of delayed control problems. Concerning the development of numerical methods and the numerical treatment of practical examples, our impression is that this topic has not yet been adequately addressed in the literature. Bader [2] applies shooting methods to the boundary value problem for the retarded state variable and the advanced adjoint variable. He successfully solves several academic examples, but his method is not capable of solving control problems with a more complicated control structure, e.g., the CSTR reactor problem described in Soliman, Ray [29, 30]. A similar CSTR reactor problem is considered in Oh, Luus [25] and Dadebo, Luus [9] who use the differential dynamic programming method with a moderate number of stages. Therefore, the second goal of this paper is the presentation of discretization and nonlinear programming methods which provide the optimal state, control and adjoint functions and allow for an accurate check of the necessary conditions.

The organization of the paper is as follows. Section 2 presents the statement of the delayed control problem with mixed state–control constraints. In section 3, we recall the minimum principle for *undelayed* control problems with control–state constraints. Here, a crucial feature is that initial and terminal boundary conditions must be considered in a general mixed form. Section 4 is devoted to the derivation of first order necessary optimality conditions for the delayed optimal control problem given in Section 2. Essentially, the augmentation approach of Guinn [13] is generalized which allows to use the minimum principle in section 3. For technical reasons, we need the assumption that the ratio of the time delays in state and control is a rational number. The analysis in this section is based on the theses of Göllmann [12] and Kern [19]. In section 5, the Euler discretization for the delayed control problem is discussed which leads to a high-dimensional nonlinear programming problem. As in the undelayed case it can be shown that the Lagrange multipliers corresponding to the optimization problem constitute a Euler discretization for the advanced adjoint equations. In section 6, we discuss an analytical example which allows to test the accuracy of the numerical solution for various stepsizes. Sections 7 and 8 are devoted to the numerical solution and the verification of the minimum principle for two practical examples. The first example is taken from [29, 30] and describes the optimal control of a chemical tank reactor (CSTR reactor), while the second example arises in the optimal harvesting of a resource (optimal fishing).

## 2 Optimal control problems with delays in state and control

We consider retarded optimal control problems with constant delays  $r \geq 0$  in the state variable  $x(t) \in \mathbb{R}^n$  and  $s \geq 0$  in the control variable  $u(t) \in \mathbb{R}^m$ . The following retarded control problem with mixed control-state inequality constraints will be referred to as problem (ROCP):

$$\text{Minimize } J(u, x) = g(x(b)) + \int_a^b L(t, x(t), x(t-r), u(t), u(t-s)) dt \quad (1)$$

subject to the retarded differential equation, boundary conditions and mixed control-state inequality constraints

$$\dot{x}(t) = f(t, x(t), x(t-r), u(t), u(t-s)), \quad \text{a.e. } t \in [a, b], \quad (2)$$

$$x(t) = \varphi(t), \quad t \in [a-r, a], \quad (3)$$

$$u(t) = \psi(t), \quad t \in [a-s, a], \quad (4)$$

$$w(x(b)) = 0, \quad (5)$$

$$C(x(t), u(t)) \leq 0, \quad t \in [a, b]. \quad (6)$$

For convenience, all functions

$$g : \mathbb{R}^n \rightarrow \mathbb{R},$$

$$L : [a, b] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R},$$

$$f : [a, b] \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^n,$$

$$w : \mathbb{R}^n \rightarrow \mathbb{R}^q, \quad 0 \leq q \leq n,$$

$$C : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^p,$$

are assumed to be twice continuously differentiable w.r.t. all arguments. A pair of functions  $(u, x) \in \mathcal{L}^\infty([a, b], \mathbb{R}^m) \times \mathcal{W}^{1,\infty}([a, b], \mathbb{R}^n)$  is called an *admissible pair* for problem (ROCP), if the state  $x$  and control  $u$  satisfy the restrictions (2)–(6). An admissible pair  $(\hat{u}, \hat{x})$  is called a *locally optimal pair* or *weak minimum* for (ROCP), if

$$J(\hat{u}, \hat{x}) \leq J(u, x)$$

holds for all  $(u, x)$  admissible in a neighborhood of  $(\hat{u}, \hat{x})$  with  $\|x(t) - \hat{x}(t)\|, \|u(t) - \hat{u}(t)\| < \varepsilon$  for all  $t \in [a, b]$  and  $\varepsilon > 0$  sufficiently small. Instead of considering a *weak minimum* we could work with the more general notion of a *Pontryagin minimum*; cf. Milyutin, Osmolovskii [22].

The Hamiltonian or Pontryagin function  $\mathcal{H}$  for the delayed control problem (ROCP) is defined in analogy to the one for nondelayed problems. However, in contrast to the nondelayed Hamiltonian, two additional arguments  $y \in \mathbb{R}^n$  and  $v \in \mathbb{R}^m$  denoting the delayed state and control variable are needed:

$$\begin{aligned} \mathcal{H}(t, x, y, u, v, \lambda, \mu) &:= L(t, x, y, u, v) + \lambda^* f(t, x, y, u, v) + \mu^* C(t, x, u), \\ \lambda &\in \mathbb{R}^n, \mu \in \mathbb{R}^p. \end{aligned} \quad (7)$$

Here and in the sequel  $*$  denotes the transposition. We shall obtain necessary optimality conditions for the retarded control problem (ROCP) by first transforming (augmenting) problem (ROCP) to a higher-dimensional nondelayed control problem. To further study the augmented problem, we need Pontryagin minimum principle for nondelayed control problems with mixed control-state constraints which will be reviewed in the next section.

### 3 First order necessary optimality conditions for undelayed optimal control problems with mixed constraints

Formally, any undelayed control problem is contained in the retarded problem (ROCP) by choosing  $r = s = 0$ . Due to the absence of delays, the initial value profiles given by

conditions (3) and (4) are omitted. However, the continuity of the state variables in the augmented problem necessitates to introduce a general boundary condition of mixed type,

$$w(x(a), x(b)) = 0, \quad (8)$$

which replaces the terminal boundary condition (5). The Hamiltonian or Pontryagin function for the nondelayed control problem is given by

$$H(t, x, u, \lambda, \mu) := L(t, x, u) + \lambda^* f(t, x, u) + \mu^* C(t, x, u). \quad (9)$$

The extension of the classical Pontryagin minimum principle to mixed control–state constraints (6) requires a regularity condition or constraint qualification. For a locally optimal pair  $(\hat{u}, \hat{x})$  and  $t \in [a, b]$ , let  $J_0(t) := \{j \in \{1, \dots, p\} \mid C_j(t, \hat{x}(t), \hat{u}(t)) = 0\}$  denote the set of active indices for the inequality constraint (6). Then we assume the rank condition:

$$\text{rank} \left( \frac{\partial C_j(t, \hat{x}(t), \hat{u}(t))}{\partial u} \right)_{j \in J_0(t)} = \#J_0(t). \quad (10)$$

The following necessary optimality conditions are to be found in Hestenes [15], Milyutin, Osmolovskii [22] and Neustadt [23].

*Theorem 3.1 (Pontryagin’s Minimum Principle.)* Let  $(\hat{u}, \hat{x})$  be a locally optimal pair for the control problem (ROCP) without delays, i.e.,  $r = s = 0$ , and the mixed boundary condition (8). Assume that the regularity condition (10) is satisfied. Then there exist a costate (adjoint) function  $\hat{\lambda} \in \mathcal{W}^{1,\infty}([a, b], \mathbb{R}^n)$ , a multiplier function  $\hat{\mu} \in \mathcal{L}^\infty([a, b], \mathbb{R}^p)$  and a multiplier  $\hat{\nu} \in \mathbb{R}^q$ , such that the following conditions hold for a.e.  $t \in [a, b]$ :

(i) adjoint differential equation:

$$\dot{\hat{\lambda}}(t)^* = -\mathcal{H}_x(t, \hat{x}(t), \hat{u}(t), \hat{\lambda}(t), \hat{\mu}(t)); \quad (11)$$

(ii) transversality conditions:

$$\hat{\lambda}(a)^* = -g_{x^\alpha}(\hat{x}(a), \hat{x}(b)) - \hat{\nu}^* w_{x^\alpha}(\hat{x}(a), \hat{x}(b)), \quad (12)$$

$$\hat{\lambda}(b)^* = g_{x^\beta}(\hat{x}(a), \hat{x}(b)) + \hat{\nu}^* w_{x^\beta}(\hat{x}(a), \hat{x}(b)); \quad (13)$$

(iii) minimum condition for the Hamiltonian function:

$$\mathcal{H}(t, \hat{x}(t), \hat{u}(t), \hat{\lambda}(t), \hat{\mu}(t)) \leq \mathcal{H}(t, \hat{x}(t), u, \hat{\lambda}(t), \hat{\mu}(t)), \quad (14)$$

for all  $u \in \mathbb{R}^m$  satisfying  $C(t, \hat{x}(t), u) \leq 0$ ;

(iv) multiplier condition and complementarity:

$$\hat{\mu}(t) \geq 0 \quad \text{and} \quad \hat{\mu}_i(t) C_i(t, \hat{x}(t), \hat{u}(t)) = 0, \quad i = 1, \dots, p. \quad (15)$$

Herein,  $g_{x^\alpha}$ ,  $g_{x^\beta}$ ,  $w_{x^\alpha}$  and  $w_{x^\beta}$  denote partial derivatives of  $g = g(x^\alpha, x^\beta)$  and  $w = w(x^\alpha, x^\beta)$  with respect to their first and second argument. In particular, the minimum condition (14) yields the local minimum condition

$$\mathcal{H}_u(t, \hat{x}(t), \hat{u}(t), \hat{\lambda}(t), \hat{\mu}(t)) = 0 \quad \text{for a.e. } t \in [a, b]. \quad (16)$$

In the next section, Theorem 3.1 will be used to derive necessary conditions for the retarded control problem (ROCP).

## 4 Necessary optimality conditions for delayed optimal control problems with mixed control-state constraints

Now we study the retarded control problem (ROCP) with constant delays  $r, s \geq 0$  and  $(r, s) \neq (0, 0)$ . We shall use a transformation technique which requires the technical assumption that the ratio of the delays is a rational number.

*Assumption 4.1 (Rationality Assumption)* Assume that  $r, s \geq 0$ ,  $(r, s) \neq (0, 0)$  and

$$\frac{r}{s} \in \mathbb{Q} \quad \text{for } s > 0, \quad \text{or} \quad \frac{s}{r} \in \mathbb{Q} \quad \text{for } r > 0. \quad (17)$$

In particular, this assumption holds for any couple of rational numbers  $(r, s)$ , where at least one number is non-zero. The following first order necessary conditions can be found in Göllmann [12]; a precise proof under Assumption 4.1. has been given by Kern [19].

*Theorem 4.2 (Minimum principle for the retarded optimal control problem (ROCP).)* Let  $(\hat{u}, \hat{x})$  be locally optimal for (ROCP) with delays satisfying Assumption 4.1. Then there exist a costate (adjoint) function  $\hat{\lambda} \in \mathcal{W}^{1,\infty}([a, b], \mathbb{R}^n)$ , a multiplier function  $\hat{\mu} \in \mathcal{L}^\infty([a, b], \mathbb{R}^p)$  and a multiplier  $\hat{\nu} \in \mathbb{R}^q$ , such that the following conditions hold for a.e.  $t \in [a, b]$ :

(i) adjoint differential equation:

$$\begin{aligned} \dot{\hat{\lambda}}(t)^* &= -\hat{\mathcal{H}}_x(t) - \chi_{[a, b-r]}(t)\hat{\mathcal{H}}_y(t+r) \\ &= -\mathcal{H}_x(t, \hat{x}(t), \hat{x}(t-r), \hat{u}(t), \hat{u}(t-s), \hat{\lambda}(t), \hat{\mu}(t)) \\ &\quad - \chi_{[a, b-r]}(t)\mathcal{H}_y(t+r, \hat{x}(t+r), \hat{x}(t), \hat{u}(t+r), \hat{u}(t+r-s), \hat{\lambda}(t+r), \hat{\mu}(t+r)), \end{aligned} \quad (18)$$

where  $\hat{\mathcal{H}}_x(t)$  and  $\hat{\mathcal{H}}_y(t)$  denote the evaluation of the partial derivatives  $\mathcal{H}_x$  and  $\mathcal{H}_y$  along  $\hat{x}(t), \hat{x}(t-r), \hat{u}(t), \hat{u}(t-s), \hat{\lambda}(t), \hat{\mu}(t)$ ;

(ii) transversality condition:

$$\hat{\lambda}(b)^* = g_x(\hat{x}(b)) + \hat{\nu}^* w_x(\hat{x}(b)); \quad (19)$$

(iii) minimum condition for the Hamiltonian function:

$$\begin{aligned} &\hat{\mathcal{H}}(t) + \chi_{[a, b-s]}(t)\hat{\mathcal{H}}(t+s) \\ &= \mathcal{H}(t, \hat{x}(t), \hat{x}(t-r), \hat{u}(t), \hat{u}(t-s), \hat{\lambda}(t), \hat{\mu}(t)) \\ &\quad + \chi_{[a, b-s]}(t)\mathcal{H}(t+s, \hat{x}(t+s), \hat{x}(t+s-r), \hat{u}(t+s), \hat{u}(t), \hat{\lambda}(t+s), \hat{\mu}(t+s)) \\ &\leq \mathcal{H}(t, \hat{x}(t), \hat{x}(t-r), u, \hat{u}(t-s), \hat{\lambda}(t), \hat{\mu}(t)) \\ &\quad + \chi_{[a, b-s]}(t)\mathcal{H}(t+s, \hat{x}(t+s), \hat{x}(t+s-r), \hat{u}(t+s), u, \hat{\lambda}(t+s), \hat{\mu}(t+s)), \end{aligned} \quad (20)$$

for all  $u \in \mathbb{R}^m$  satisfying  $C(t, \hat{x}(t), u) \leq 0$ ;

(iv) multiplier condition and complementarity condition:

$$\hat{\mu}(t) \geq 0 \quad \text{and} \quad \hat{\mu}_i(t) C_i(t, \hat{x}(t), \hat{u}(t)) = 0, \quad i = 1, \dots, p. \quad (21)$$

*Proof.* The proof uses a transformation technique suggested by Guinn [13] to derive first order necessary conditions for unconstrained optimal control problems with pure state delays. In view of the rationality assumption (17) there exists integers  $k, l \in \mathbb{N}$  with

$$\frac{r}{s} = \frac{k}{l} \quad \text{for } s \neq 0, \quad \frac{s}{r} = \frac{l}{k} \quad \text{for } r \neq 0.$$

Without loss of generality we may assume the first case. Then the delays  $r, s$  are integer multiples of the interval length  $h := s/l$ ,

$$r = k \cdot h, \quad s = l \cdot h, \quad k, l \in \mathbb{N}.$$

The time interval  $[a, a+h]$  will be used below as the basis time interval for the augmented control problem. Without loss of generality we may further assume that the interval length  $b-a$  represents an integer multiple of  $h$ , i.e., we have  $b-a = Nh$  with  $N \in \mathbb{N}_+$ .

Now we introduce the state variable  $\Xi^* = (\xi_0^*, \dots, \xi_{N-1}^*) \in \mathbb{R}^{Nn}$ ,  $\xi_i \in \mathbb{R}^n$ , and control variable  $\Theta^* = (\theta_0^*, \dots, \theta_{N-1}^*) \in \mathbb{R}^{Nm}$ ,  $\theta_i \in \mathbb{R}^m$ , which are defined by

$$\xi_i(t) := x(t + ih), \quad \theta_i(t) := u(t + ih), \quad \text{for } t \in [a, a+h], \quad i = 0, \dots, N-1. \quad (22)$$

The continuity of the state  $x(t)$  in  $[a, b]$  implies the following boundary conditions for the augmented state  $\Xi(t)$ ,

$$\xi_i(a+h) = \xi_{i+1}(a), \quad i = 0, \dots, N-2,$$

which can be written as

$$V_i(\xi_{i+1}(a), \xi_i(a+h)) := \xi_i(a+h) - \xi_{i+1}(a) = 0, \quad i = 0, \dots, N-2. \quad (23)$$

In terms of the new state and control variables  $\Xi$  and  $\Theta$ , the retarded control problem (ROCP) is equivalent to the following undelayed optimal control problem on the time interval  $[a, a+h]$ :

$$\text{Minimize } J(\Theta, \Xi) = g(\xi_{N-1}(a+h)) + \int_a^{a+h} \sum_{i=0}^{N-1} L(t+ih, \xi_i(t), \xi_{i-k}(t), \theta_i(t), \theta_{i-l}(t)) dt \quad (24)$$

subject to

$$\dot{\xi}_i(t) = f(t+ih, \xi_i(t), \xi_{i-k}(t), \theta_i(t), \theta_{i-l}(t)), \quad i = 0, \dots, N-1, \quad t \in [a, a+h], \quad (25)$$

$$\begin{aligned} V_i(\xi_{i+1}(a), \xi_i(a+h)) &= 0, \quad i = 0, \dots, N-2, \\ V_{N-1}(\xi_{N-1}(a+h)) &:= w(\xi_{N-1}(a+h)) = 0, \end{aligned} \quad (26)$$

$$C(t+ih, \xi_i(t), \theta_i(t)) \leq 0, \quad i = 0, \dots, N-1, \quad t \in [a, a+h]. \quad (27)$$

The fixed starting profiles (3) and (4) are included in this notation by considering the variables  $\xi_{-k}, \dots, \xi_{-1}$  and  $\theta_{-l}, \dots, \theta_{-1}$  defined by

$$\begin{aligned} \xi_i(t) &:= \varphi(t+ih), \quad i = -k, \dots, -1, \\ \theta_i(t) &:= \psi(t+ih), \quad i = -l, \dots, -1. \end{aligned}$$



However, note that  $\xi_{-k}, \dots, \xi_{-1}$  and  $\theta_{-l}, \dots, \theta_{-1}$  do not represent optimization variables. Introducing adjoint variables and multipliers for the augmented problem by (24)–(27) by

$$\Lambda = (\Lambda_0, \dots, \Lambda_{N-1})^* \in \mathbb{R}^{N \cdot n}, \quad M = (M_0, \dots, M_{N-1})^* \in \mathbb{R}^{N \cdot p},$$

the Hamiltonian (9) for the nondelayed augmented control problem is given by

$$\begin{aligned} \mathcal{K}(t, \Xi, \Theta, \Lambda, M) = & \sum_{i=0}^{N-1} [L(t + ih, \xi_i, \xi_{i-k}, \theta_i, \theta_{i-l}) + \Lambda_i^* L(t + ih, \xi_i, \xi_{i-k}, \theta_i, \theta_{i-l})] \\ & + \sum_{i=0}^{N-1} M_i^* C(t + ih, \xi_i, \theta_i). \end{aligned} \quad (28)$$

Every locally optimal pair  $(\hat{u}(\cdot), \hat{x}(\cdot))$  for (ROCP) defines a pair  $(\hat{\Theta}(\cdot), \hat{\Xi}(\cdot))$  that minimizes the augmented problem (24)–(27). Pontryagin's minimum principle for nondelayed problems (Theorem 3.1) assures the existence of a costate (adjoint) function  $\hat{\Lambda} \in \mathcal{W}^{1,\infty}([a, a+h], \mathbb{R}^{N \cdot n})$ , a multiplier function  $\hat{M} \in \mathcal{L}^\infty([a, a+h], \mathbb{R}^{N \cdot p})$  and a vector  $\nu \in \mathbb{R}^{(N-1)n+q}$ ,  $\hat{\nu} = (\hat{\nu}_0^*, \dots, \hat{\nu}_{N-2}^*, \hat{\nu}_{N-1}^*)^*$  where  $\hat{\nu}_0, \dots, \hat{\nu}_{N-2} \in \mathbb{R}^n$  and  $\hat{\nu}_{N-1} \in \mathbb{R}^q$ , such that the following conditions hold for almost every  $t \in [a, a+h]$ :

1. *adjoint differential equation:*

$$\frac{d}{dt} \hat{\Lambda}(t)^* = -\mathcal{K}_\Xi(t, \hat{\Xi}(t), \hat{\Theta}(t), \hat{\Lambda}(t), \hat{M}(t)); \quad (29)$$

2. *transversality condition:*

$$\hat{\Lambda}_i(a)^* = -\hat{\nu}_i^* \frac{\partial}{\partial \xi_i} V_i(\hat{\xi}_{i+1}(a), \hat{\xi}_i(a+h)), \quad i = 0, \dots, N-2, \quad (30)$$

$$\hat{\Lambda}_i(a+h)^* = \hat{\nu}_i^* \frac{\partial}{\partial \xi_{i+1}} V_i(\hat{\xi}_{i+1}(a), \hat{\xi}_i(a+h)), \quad i = 0, \dots, N-2, \quad (31)$$

$$\hat{\Lambda}_{N-1}(a+h)^* = g_x(\hat{\xi}_{N-1}(a+h)) + \hat{\nu}_{N-1}^* w_x(\hat{\xi}_{N-1}(a+h)); \quad (32)$$

3. *minimum condition for the Hamiltonian:*

$$\mathcal{K}(t, \hat{\Xi}(t), \hat{\Theta}(t), \hat{\Lambda}(t), \hat{M}(t)) \leq \mathcal{K}(t, \hat{\Xi}(t), \Theta, \hat{\Lambda}(t), \hat{M}(t)) \quad (33)$$

for all admissible  $\Theta = (\theta_0^*, \dots, \theta_{N-1}^*)^* \in \mathbb{R}^{N \cdot m}$  with  $C(t + ih, \hat{\xi}_i(t), \theta_i) \leq 0$  and  $i = 0, \dots, N-1$ ;

4. *multiplier condition and complementarity:*

$$\hat{M}(t) \geq 0, \quad \hat{M}_i(t)^* C(t + ih, \hat{\xi}_i(t), \hat{\theta}_i(t)) = 0, \quad i = 0, \dots, N-1. \quad (34)$$

Evaluating the adjoint equation for the component  $\hat{\Lambda}_j$ , ( $0 \leq j \leq N-1$ ) yields

$$\begin{aligned} \frac{d}{dt} \hat{\Lambda}_j(t)^* = & -L_x(t + jh, \hat{\xi}_j(t), \hat{\xi}_{j-k}(t), \hat{\theta}_j(t), \hat{\theta}_{j-l}(t)) \\ & - \chi_{\{0, \dots, N-1-k\}}(j) L_y(t + (j+k)h, \hat{\xi}_{j+k}(t), \hat{\xi}_j(t), \hat{\theta}_{j+k}(t), \hat{\theta}_{j+k-l}(t)) \\ & - \hat{\Lambda}_j(t)^* f_x(t + jh, \hat{\xi}_j(t), \hat{\xi}_{j-k}(t), \hat{\theta}_j(t), \hat{\theta}_{j-l}(t)) \\ & - \chi_{\{0, \dots, N-1-k\}}(j) \hat{\Lambda}_{j+k}(t)^* L_y(t + (j+k)h, \hat{\xi}_{j+k}(t), \hat{\xi}_j(t), \hat{\theta}_{j+k}(t), \hat{\theta}_{j+k-l}(t)) \\ & - \hat{M}_j(t)^* C_x(t + jh, \hat{\xi}_j(t), \hat{\theta}_j(t)). \end{aligned}$$

Now we are able to define the adjoint function  $\hat{\lambda} \in \mathcal{W}^{1,\infty}([a, b], \mathbb{R}^n)$  and multiplier function  $\hat{\mu} \in \mathcal{L}^\infty([a, b], \mathbb{R}^p)$  for the retarded control problem (ROCP) in the following way. For  $t \in [a, b]$  there exists  $0 \leq j \leq N - 1$  with  $a + jh \leq t \leq a + (j + 1)h$ . We put

$$\hat{\lambda}(t) := \hat{\Lambda}_j(t - jh), \quad \hat{\mu}(t) := \hat{M}(t - jh) \quad (35)$$

and obtain from the previous adjoint equation:

$$\begin{aligned} \dot{\hat{\lambda}}(t) &= \frac{d}{dt} \hat{\Lambda}_j(t - jh) \\ &= -L_x(t, \hat{x}(t), \hat{x}(t - kh), \hat{u}(t), \hat{u}(t - lh)) \\ &\quad - \chi_{\{0, \dots, N-1-k\}}(j) L_y(t + kh, \hat{x}(t + kh), \hat{x}(t), \hat{u}(t + kh), \hat{u}(t + kh - lh)) \\ &\quad - \hat{\lambda}(t)^* f_x(t, \hat{x}(t), \hat{x}(t - kh), \hat{u}(t), \hat{u}(t - lh)) \\ &\quad - \chi_{\{1, \dots, N-1-k\}}(j) \hat{\lambda}(t + kh)^* f_y(t + kh, \hat{x}(t + kh), \hat{x}(t), \hat{u}(t + kh), \hat{u}(t + kh - lh)) \\ &\quad - \hat{\mu}(t)^* C_x(t, \hat{x}(t), \hat{u}(t)) \\ &= -\mathcal{H}(t, \hat{x}(t), \hat{x}(t - r), \hat{u}(t), \hat{u}(t - s), \hat{\lambda}(t), \hat{\mu}(t)) \\ &\quad - \chi_{[a, b-r]}(t) \mathcal{H}(t + r, \hat{x}(t + r), \hat{x}(t), \hat{u}(t + r), \hat{u}(t + r - s), \hat{\lambda}(t + r) \hat{\mu}(t + r)). \end{aligned}$$

Thus we have found the adjoint equation (18). The transversality condition (32) for  $\Lambda_{N-1}$ ,

$$\hat{\Lambda}_{N-1}(a + h)^* = g_x(\hat{\xi}_{N-1}(a + h)) + \hat{\nu}_{N-1}^* w_x(\hat{\xi}_{N-1}(a + h)),$$

gives the desired transversality condition (19) for (ROCP) in view of  $b = a + Nh$ :

$$\hat{\lambda}(a + Nh) = g_x(\hat{x}(a + Nh)) + \hat{\nu}^* w_x(\hat{x}(a + Nh)), \quad \hat{\nu} := \hat{\nu}_{N-1} \in \mathbb{R}^q.$$

To verify the minimum condition for the Hamiltonian  $\mathcal{H}$ , we consider  $t \in [a, b]$  and the corresponding index  $j \in \{0, \dots, N - 1\}$  with  $a + jh \leq t \leq a + (j + 1)h$ . Putting  $t' := t - jh \in [a, a + h]$ , the minimum condition (33) gives

$$\mathcal{K}(t', \hat{\Xi}(t'), \hat{\Theta}(t'), \hat{\Lambda}(t'), \hat{M}(t')) \leq \mathcal{K}(t', \hat{\Xi}(t'), \Theta, \hat{\Lambda}(t'), \hat{M}(t')), \quad (36)$$

for all admissible  $\Theta \in \mathbb{R}^{Nm}$ . We now define an admissible control policy  $\Theta(\cdot) = (\theta_0^*, \dots, \theta_{N-1}^*)^* \in \mathbb{R}^{Nm}$  by

$$\theta_i := \begin{cases} \hat{u}(t' + ih), & i \neq j \\ u, & i = j \end{cases}, \quad i = 0, \dots, N - 1,$$

where the control vector  $u \in \mathbb{R}^m$  is admissible for (ROCP), i.e.,  $C(t, \hat{x}(t), u) \leq 0$ . Evaluating the inequality (36) for this vector  $\Theta$  and removing equal expressions on both sides, we get for the remaining terms associated with  $j$  and  $j + l$ :

$$\begin{aligned}
& L(t' + jh, \hat{\xi}_j(t'), \hat{\xi}_{j-k}(t'), \hat{u}(t' + jh), \hat{u}(t' + (j-l)h)) \\
& + \hat{\Lambda}_j(t')^* f(t' + jh, \hat{\xi}_j(t'), \hat{\xi}_{j-k}(t'), \hat{u}(t' + jh), \hat{u}(t' + (j-l)h)) \\
& + \hat{M}_j(t')^* C(t', \hat{\xi}_j(t'), \hat{u}(t' + jh)) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) L(t' + (j+l)h, \hat{\xi}_{j+l}(t'), \hat{\xi}_{j+l-k}(t'), \hat{u}(t' + (j+l)h), \hat{u}(t' + jh)) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) \hat{\Lambda}_{j+l}(t')^* f(t' + (j+l)h, \hat{\xi}_{j+l}(t'), \hat{\xi}_{j+l-k}(t'), \hat{u}(t' + (j+l)h), \hat{u}(t' + jh)) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) \hat{M}_{j+l}(t')^* C(t', \hat{\xi}_{j+l}(t'), \hat{u}(t' + (j+l)h)) \\
\leq & L(t' + jh, \hat{\xi}_j(t'), \hat{\xi}_{j-k}(t'), u, \hat{u}(t' + (j-l)h)) \\
& + \hat{\Lambda}_j(t')^* f(t' + jh, \hat{\xi}_j(t'), \hat{\xi}_{j-k}(t'), u, \hat{u}(t' + (j-l)h)) \\
& + \hat{M}_j(t')^* C(t', \hat{\xi}_j(t'), u) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) L(t' + (j+l)h, \hat{\xi}_{j+l}(t'), \hat{\xi}_{j+l-k}(t'), \hat{u}(t' + (j+l)h), u) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) \hat{\Lambda}_{j+l}(t')^* f(t' + (j+l)h, \hat{\xi}_{j+l}(t'), \hat{\xi}_{j+l-k}(t'), \hat{u}(t' + (j+l)h), u) \\
& + \chi_{\{0, \dots, N-1-l\}}(j) \hat{M}_{j+l}(t')^* C(t', \hat{\xi}_{j+l}(t'), \hat{u}(t' + (j+l)h))
\end{aligned}$$

Redefining the functions according to (35), we obtain the desired minimum condition (20) for  $\mathcal{H}$  since  $t' = t - jh$ . Condition (34) immediately implies the multiplier and complementarity condition (21) in view of (35).  $\square$

**Remark:** Soliman, Ray [30] have discussed bang-bang and singular controls which appear in control problems, where the control  $u \in \mathbb{R}^m$  is partitioned into controls  $u_1 \in \mathbb{R}^{m_1}$  and  $u_2 \in \mathbb{R}^{m_2}$  with control  $u_1$  appearing *linearly* in the system. The control-state constraint (6) then reduces to bounds for  $u_1$ ,

$$u_{1,min} \leq u_1(t) \leq u_{1,max} \quad \text{for } t \in [a, b], \quad u_{1,min}, u_{1,max} \in \mathbb{R}^{m_1}.$$

The minimum condition (20) shows that the control  $u_1(t)$  is determined by the sign of the components of the *switching vector function*

$$\sigma(t) = \mathcal{H}_{u_1}(t) + \chi_{[a,b]}(t+s) \mathcal{H}_{v_1}(t+s), \quad (37)$$

while the control  $u_2$  satisfies the equation

$$0 = \mathcal{H}_{u_2}(t) + \chi_{[a,b]}(t+s) \mathcal{H}_{v_2}(t+s). \quad (38)$$

The CSTR control problem in section 6 provides an example with such a partitioning of the control vector. Soliman, Ray [30] study junction phenomena for bang-bang and singular arcs. They give conditions under which junction results for control systems without delay carry over to delayed systems, but also give examples for delayed systems which exhibit unusual features which require further work to develop fully the theory. Further examples illustrating these unusual features have been worked out by Kern [19].

## 5 Discretization, optimization and the consistency of adjoint variables

Without restrictions we may assume that the cost functional for the retarded control problem (ROCP) is given in Mayer form

$$J(u, x) = g(x(b)).$$

The reduction of the more general cost functional (1) to Mayer form proceeds as for undelayed control systems by introduction of the additional state variable  $x_0$  through the retarded equation

$$\dot{x}_0(\tau) = L(t, x(t), x(t-r), u(t), u(t-s)), \quad x_0(a) = 0.$$

Then the cost functional (1) is rewritten in Mayer form  $J(u, \tilde{x}) = g(x(b)) + x_0(b)$  with the new state variable  $\tilde{x} = (x_0, x^*) \in \mathbb{R}^{n+1}$ .

As for undelayed differential equations, there exist standard integration schemes of Euler or Runge–Kutta type for the retarded differential equation  $\dot{x}(t) = f(t, x(t), x(t-r), u(t), u(t-s))$ . Using an uniform stepsize  $h > 0$ , it is crucial to match the delays  $r$  and  $s$  to the stepsize  $h$  by the following assumption:

$$\frac{r}{h} = k \in \mathbb{N}, \quad \frac{s}{h} = l \in \mathbb{N}. \quad (39)$$

Note that, if  $h$  satisfies (39), any fraction  $h/\nu$  with  $\nu \in \mathbb{N}$  also does. Therefore, the restriction (39) is satisfied for all finer grids. For simplicity, we discuss Euler's integration method with stepsize  $h = (b-a)/N$  for  $N \in \mathbb{N}_+$  and grid points  $t_i = a + ih$ ,  $i = 0, 1, \dots, N$ . Using the approximations  $x(t_i) \approx x_i \in \mathbb{R}^n$ ,  $u(t_i) \approx u_i \in \mathbb{R}^m$ , we obtain the following nonlinear programming problem (NLP):

$$\text{Minimize} \quad J(u, x) = g(x_N) \quad (40)$$

subject to

$$-x_{i+1} + x_i + hf(t_i, x_i, x_{i-k}, u_i, u_{i-l}) = 0, \quad i = 0, \dots, N-1, \quad (41)$$

$$x_{-i} = \varphi(a - ih), \quad i = 0, \dots, k, \quad (42)$$

$$u_{-i} = \psi(a - ih), \quad i = 1, \dots, l, \quad (43)$$

$$w(x_N) = 0, \quad (44)$$

$$C(t_i, x_i, u_i) \leq 0, \quad i = 0, \dots, N. \quad (45)$$

The optimization variable in (NLP) is represented by the vector

$$z := (u_0, x_0, u_1, x_1, \dots, u_N, x_N) \in \mathbb{R}^{(N+1)(m+n)}.$$

The necessary optimality conditions for (NLP) by Karush–Kuhn–Tucker yield Lagrange multipliers  $\hat{\lambda}_i \in \mathbb{R}^n$  ( $i = 0, \dots, N-1$ ) for the equation (41), a multiplier  $\hat{\mu}_i \in \mathbb{R}^p$  ( $i = 0, \dots, N$ ) for the inequality constraint (45) and a multiplier  $\nu \in \mathbb{R}^q$  for the boundary condition (44). Upon defining the multiplier  $\hat{\lambda}_N := g_x(\hat{x}_N) + \nu_N^* w_x(\hat{x}_N)$ , it is straightforward to verify that the following approximations hold:

$$\hat{\lambda}(t_i) \approx \tilde{\lambda}_i, \quad \hat{\mu}(t_i) \approx \frac{1}{h} \hat{\mu}_i \quad (i = 0, \dots, N), \quad \hat{\nu} \approx \hat{\nu}_N. \quad (46)$$

The important point to note here is the proper scaling of the multiplier  $\hat{\mu}_i \in \mathbb{R}^p$ . The multipliers  $\hat{\lambda}_i \in \mathbb{R}^n$  ( $i = 0, \dots, N - 1$ ) can be identified as solutions to the discretized advanced adjoint equation (18) with boundary condition (19).

To solve the optimization problem (NLP) in (40) – (45), we employ the programming language AMPL in Fourer, Gay and Kernighan [11] together with the optimization solvers LOQO developed by Vanderbei [31] or IPOPT by Wächter et al. [33, 34]. Both solvers also provide the Lagrange multipliers and hence a discretization of the adjoint variables for the control problem (ROCP). Alternatively, the optimization problem (NLP) can be solved using the code NUDOCCS developed by Büskens [4]. Instead of Euler’s discretization scheme we also may use any Runge–Kutta type integration scheme of an order less than four.

For notational ease in the following examples, we suppress the “hat” to denote optimal solutions.

## 6 An analytical example

We consider the following optimal control problem with the delay  $r = 1$  in the state and  $s = 2$  in the control:

$$\text{Minimize } \int_0^3 (x^2(t) + u^2(t)) dt \quad (47)$$

subject to

$$\dot{x}(t) = x(t - 1)u(t - 2), \quad t \in [0, 3], \quad (48)$$

$$x(t) = 1, \quad t \in [-1, 0], \quad (49)$$

$$u(t) = 0, \quad t \in [-2, 0]. \quad (50)$$

A control-state constraint will be imposed later. The Hamiltonian (7) for this problem is

$$\mathcal{H}(t, x, y, u, v) = x^2 + u^2 + \lambda y v. \quad (51)$$

For an optimal pair  $(u, x)$ , the adjoint equations (18) in Theorem 4.2 yield

$$\begin{aligned} \dot{\lambda}(t) &= -\mathcal{H}_x(t, x(t), x(t - 1), u(t), u(t - 2), \lambda(t)) \\ &\quad -\chi_{[0,2]}(t)\mathcal{H}_y(t + 1, x(t + 1), x(t), u(t + 1), u(t - 1), \lambda(t + 1)) \\ &= -2x(t) - \chi_{[0,2]}(t)\lambda(t + 1)u(t - 1). \end{aligned}$$

It immediately follows from (48)–(50) that

$$x(t) = 1 \quad \text{for } t \in [0, 2].$$

The state variable can only be influenced by the control  $u(t - 2)$  on the terminal interval  $[2, 3]$ . Hence, it suffices to determine the optimal control  $u(t)$  on the interval  $[0, 1]$ . The minimum condition (20) requires the minimization of the expression

$$\mathcal{H}(t, x(t), x(t - 1), u, u(t - 2)) + \chi_{[0,1]}(t)\mathcal{H}(t + 2, x(t + 2), x(t + 1), u(t + 2), u)$$

w.r.t. the control variable  $u$  for  $t \in [0, 3]$ . For  $t \in [0, 1]$ , we obtain  $2u(t) + \lambda(t + 2)x(t + 1) = 0$ , which yields the control

$$u(t) = -\frac{1}{2}\lambda(t + 2)x(t + 1) = -\frac{1}{2}\lambda(t + 2), \quad t \in [0, 1].$$

On the interval  $[1, 3]$ , we immediately get

$$u(t) = 0 \quad \text{for } t \in [1, 3].$$

Then on  $[2, 3]$ , the adjoint and state equation become

$$\dot{\lambda}(t) = 2x(t) - 2u(t) = 2x(t), \quad \dot{x}(t) = u(t - 2) = -\frac{1}{2}\lambda(t - 2 + 2) = -\frac{1}{2}\lambda(t).$$

This yields a second order differential equation for  $\lambda$ ,

$$\ddot{\lambda}(t) = -2\dot{x}(t) = \lambda(t), \quad \text{for } t \in [2, 3],$$

which has the general solution

$$\lambda(t) = Ae^t + Be^{-t}, \quad x(t) = -\frac{1}{2}(Ae^t - Be^{-t}).$$

The constants  $A$  and  $B$  can be determined from the transversality condition (19) and the continuity of the state  $x(t)$  at  $t = 2$ ,

$$\lambda(3) = 0, \quad x(2) = 1,$$

from which we find

$$A = \frac{-2e^{-2}}{e^2 + 1}, \quad B = \frac{2e^4}{e^2 + 1}.$$

Then the control  $u$  on the first segment  $[0, 1]$  is given by

$$u(t) = \frac{e^{-2}}{e^2 + 1}e^{t+2} - \frac{e^4}{e^2 + 1}e^{-(t+2)} \quad \text{for } t \in [0, 1].$$

Now we evaluate the costate on the second interval  $[1, 2]$ . The advanced differential equation

$$\begin{aligned} \dot{\lambda}(t) &= -2x(t) - \lambda(t+1)u(t-1) = -2 + \frac{1}{2}(\lambda(t+1))^2 \\ &= -2 + \frac{1}{2} \left( \frac{-2e^{-2}}{e^2 + 1}e^{t+1} + \frac{2e^4}{e^2 + 1}e^{-(t+1)} \right)^2 \end{aligned}$$

and the continuity of the costate,  $\lambda(2^-) = \lambda(2^+) = \frac{2(e^2-1)}{e^2+1} \approx 1.523188311$ , yield the explicit solution

$$\begin{aligned} \lambda(t) &= \lambda(2^+) + \int_2^t \left( -2 + \frac{1}{2}(\lambda(\tau+1))^2 \right) d\tau \\ &= \frac{e^{2t-2} - e^{6-2t}}{(e^2 + 1)^2} - t \cdot \left( \frac{4e^2}{(e^2 + 1)^2} + 2 \right) + \frac{4(e^2 - 1)}{(e^2 + 1)^2} + 6 \quad \text{for } t \in [1, 2]. \end{aligned}$$

Similarly, we can compute  $\lambda(t)$  on  $[0, 1]$ . Since  $x(t) = 1$  and  $u(t) = 0$  on  $[0, 1]$ , the adjoint equation reduces to

$$\dot{\lambda}(t) = -2x(t) - \lambda(t+1)u(t-1) = -2.$$

Then the continuity of  $\lambda$  in  $t = 1$ ,  $\lambda(1^-) = \lambda(1^+) = \frac{2(e^2-1)}{(e^2+1)^2} + 3 \approx 3.181568497$ , leads to the following representation

$$\lambda(t) = \lambda(1^+) + 2 - 2t = -2t + \frac{2(e^2 - 1)}{(e^2 + 1)^2} + 5 \quad \text{for } t \in [0, 1].$$

Summing up our findings, we have obtained the optimal solution  $(x, u, \lambda)$ :

$$\text{for } t \in [0, 1]: \quad x(t) = 1, \quad u(t) = \frac{e^{-2}}{e^2 + 1}e^{t+2} - \frac{e^4}{e^2 + 1}e^{-(t+2)},$$

$$\lambda(t) = -2t + \frac{2(e^2 - 1)}{(e^2 + 1)^2} + 5,$$

$$\text{for } t \in [1, 2]: \quad x(t) = 1, \quad u(t) = 0,$$

$$\lambda(t) = \frac{e^{2t-2} - e^{6-2t}}{(e^2 + 1)^2} - t \cdot \left( \frac{4e^2}{(e^2 + 1)^2} + 2 \right) + \frac{4(e^2 - 1)}{(e^2 + 1)^2} + 6,$$

$$\text{for } t \in [2, 3]: \quad x(t) = \frac{e^{-2}}{e^2 + 1}e^t + \frac{e^4}{e^2 + 1}e^{-t}, \quad u(t) = 0, \quad \lambda(t) = \frac{-2e^{-2}}{e^2 + 1}e^t + \frac{2e^4}{e^2 + 1}e^{-t}.$$

The analytical optimal solution allows us to determine the optimal performance index explicitly after some lengthy computations:

$$J = \int_0^3 (x^2(t) + u^2(t)) dt = \frac{3}{2} - \frac{3e^2 + 1}{(e^2 + 1)^2} + 1 + \frac{e^4 + 4e^2 - 1}{2(e^2 + 1)^2} = 3 - \frac{2}{e^2 + 1} \approx 2.76159.$$

Let us now compare the analytical solution with the numerical results which are obtained by applying the discretization and optimization methods in section 5. We solve the Euler-discretized nonlinear optimization problem (40) – (43) using the interior-point code IPOPT developed by Wächter et al. [33, 34] with error tolerance  $\text{tol} = 10^{-10}$ . The starting solution is  $x(t) \equiv 1$  and  $u(t) \equiv 0$ . Using a coarse discretization with  $N = 600$  grid points, we find the performance index  $J(x, u) = 2.765928244$  in 0.0127 CPU seconds. This value means a deviation of about 0.16% from the analytical value  $J = 2.761594156$ . Increasing the discretization by a factor 100, i.e., using  $N = 60000$  gridpoints, we get  $J(x, u) = 2.761638$  in 2.5 CPU seconds. The extremely fine discretization with  $N = 480000$  gridpoints yields  $J(x, u) = 2.761599$  which is correct in 5 decimals. In Fig. 1, the numerical solution trajectories for a mesh of  $N = 600$  grid points are presented.

Next, we impose the mixed control-state-constraint

$$u(t) + x(t) \geq 0.3 \quad \text{for } t \in [0, 6]. \quad (52)$$

We have doubled the length of the time interval to get a more interesting structure of boundary arcs for the mixed control-state constraint. Here, it is not possible any more to determine an optimal solution analytically. Again, we use an Euler discretization with  $N = 600$  or  $N = 60000$  grid points. The numerical results for the optimal state, the optimal control and the adjoint variable arising from a mesh size of  $N = 600$  points are displayed in Fig. 2. The constraint function  $x(t) + u(t)$  and the corresponding multiplier  $\mu(t)$  are presented in Fig. 3.

The performance index for  $N = 600$  is  $J(x, u) = 3.121827278$  with CPU = 0.32 sec, while  $N = 60000$  gives  $J(x, u) = 3.108259352$  with CPU = 65.8 sec. The necessary optimality conditions in Theorem 4.2 provide the existence of a multiplier function  $\hat{\mu}$  satisfying

$$\mu(t) \geq 0, \quad \mu(t)(0.3 - u(t) - x(t)) = 0 \quad \text{for } t \in [0, 6]. \quad (53)$$

Fig. 3 clearly shows that the computed multiplier does satisfy this condition. We have two boundary arcs  $[0, t_1]$ ,  $t_1 \approx 0.46$ , and  $[t_2, 6]$ ,  $t_2 \approx 3.18$ , where the control-state constraint becomes active. In the interior of the boundary arcs, the multiplier  $\mu(t)$  is strictly positive, while  $\mu(t)$  vanishes on the interior arc.

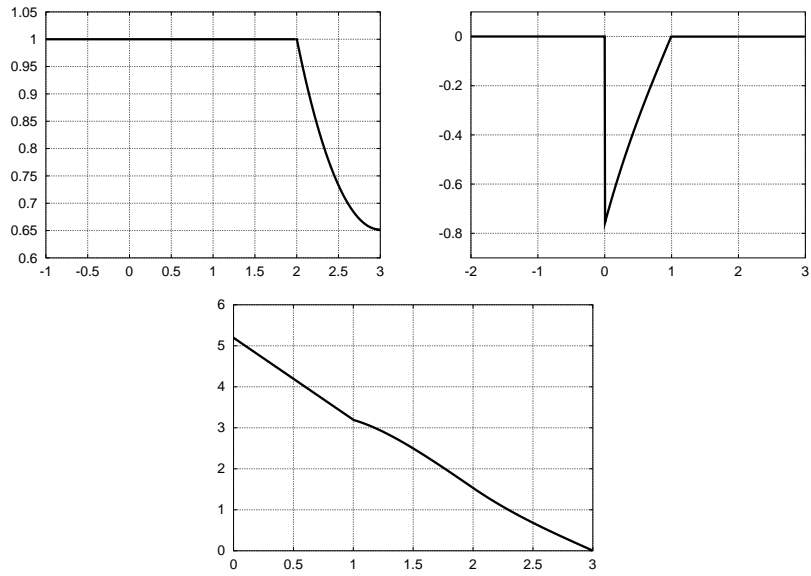


Figure 1: Optimal state  $x(t)$ , control  $u(t)$  and adjoint  $\lambda(t)$  determined numerically ( $N=600$ ).

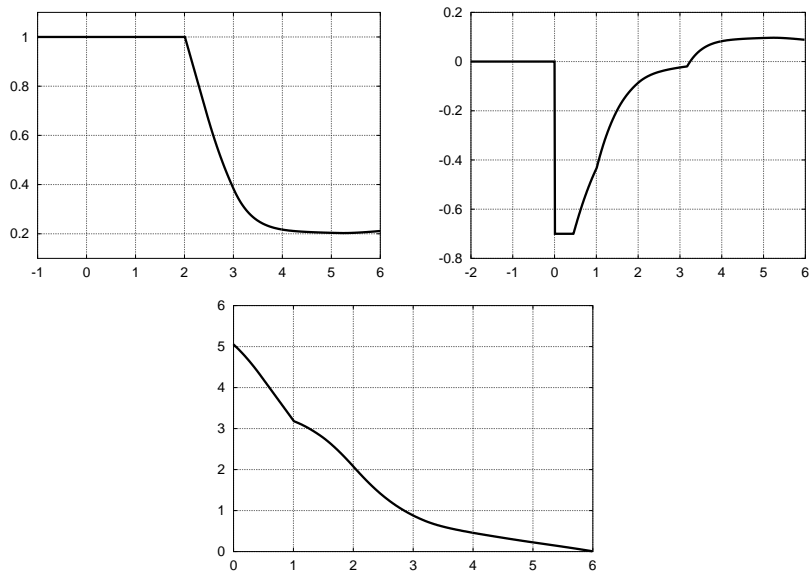


Figure 2: Control–state constraint  $0.3 \leq x(t) + u(t)$ : optimal state  $x(t)$ , control  $u(t)$  and adjoint  $\lambda(t)$ .



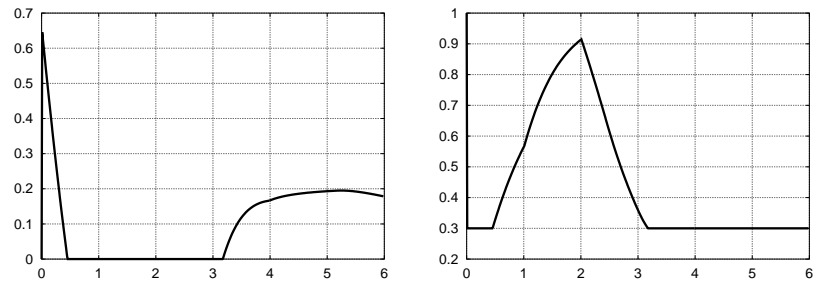


Figure 3: Control–state constraint  $0.3 \leq x(t) + u(t)$ : multiplier  $\mu(t)$  and function  $x(t) + u(t)$ .

## 7 A nonlinear chemical tank reactor model

We consider a continuous nonlinear stirred tank reactor system (CSTR) that runs an irreversible chemical reaction. The model is taken from Soliman and Ray [27, 29]; cf. also Bader [2]. The process is described by the relative concentration  $x_1$  of the product, the relative concentration  $x_2$  of the catalyst and the relative temperature in the reaction vessel. All these quantities represent the relative deviation to an equilibrium and thus held completely dimensionless. This model is based upon earlier work by Soliman and Ray [27] and has been slightly modified. The chemical agents in the vessel are stirred by an

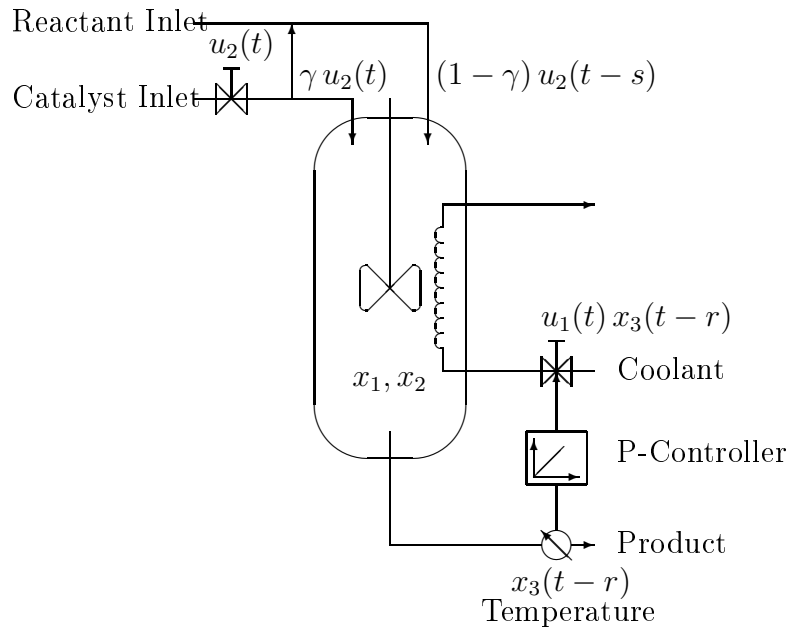


Figure 4: Continuous stirred tank reactor (CSTR) after Soliman and Ray.

agitator and thus kept in a permanent movement. The reaction is steered by two control functions. The catalyst feed is split into a fraction  $\gamma u_2(t)$  entering the vessel directly and a remaining fraction  $(1 - \gamma) u_2(t - s)$  entering the vessel with a time delay  $r$  due to prior mixing with the reactant feed. The temperature inside the vessel is controlled by a function  $u_1(t)$  representing a time dependent proportional gain of a heat exchanger device. The adjustment of the temperature depends on a feedback p-controller that depends on the outlet temperature  $x_3(t - r)$ .

Our goal is to transfer the system in a balance within a fixed time interval optimally. The objective functional essentially represents the deviation of the state to its equilibrium.

Problem (CSTR) Minimize

$$J(u, x) = \int_0^{0.2} (\|x(t)\|_2^2 + 0.01u_2^2(t))dt$$

subject to

$$\begin{aligned}\dot{x}_1(t) &= -x_1(t) - R(t), \\ \dot{x}_2(t) &= -x_2(t) + 0.9u_2(t-s) + 0.1u_2(t), \\ \dot{x}_3(t) &= -2x_3(t) + 0.25R(t) - 1.05u_1(t)x_3(t-r),\end{aligned}$$

for a.e.  $t \in [0, 0.2]$ , where

$$R(t) = R(t, x_1(t), x_2(t), x_3(t)) := (1 + x_1(t))(1 + x_2(t)) \exp\left(\frac{25x_3(t)}{1 + x_3(t)}\right),$$

and the initial and terminal conditions, resp., control constraint

$$\begin{aligned}x_3(t) &= -0.02, & t \in [-r, 0), \\ u_2(t) &= 1, & t \in [-s, 0), \\ x(0) &= (0.49, -0.0002, 0.02)^*, \\ x(0.2) &= (0, 0, 0)^*, \\ |u_1(t)| &\leq 500, & t \in [0, 0.2].\end{aligned}$$

We choose the state delay  $r = 0.015$  and control delay  $s = 0.02$ . Bader [2] attempted to solve this CSTR problem by using shooting methods. However, due to the complicated structure of the control, Bader could only obtain a coarse approximation of the optimal solution. We solve the discretized control problem (NLP) in section 5 by utilizing the Interior Point code IPOPT. The numerical computations have been carried out with  $N = 16000$  grid points. We obtain an optimized performance index of  $J = 0.011970541$ . Due to the fixed terminal condition for the state  $x(0.2)$  the algorithm requires the rather vast amount of 63,932 seconds of CPU time. One can expect an acceleration by considering a free terminal state instead and a quadratically appearing control component  $u_1$  in the objective functional. The computed optimal solution and the adjoint variables  $\lambda_1, \lambda_2$ , and  $\lambda_3$  are shown in figs. 5 – 7.

Let us discuss the minimum principle in Theorem 4.2 in greater detail. Since there are no mixed control-state constraints, the Hamiltonian function (7) is given by

$$\begin{aligned}\mathcal{H}(t, x_1, x_2, x_3, y_3, \lambda, u_1, u_2, v_2) &= \|x\|_2^2 + 0.01u_2^2 + \lambda_1(-x_1 - R(x)) \\ &+ \lambda_2(-x_2 + 0.9v_2 + 0.1u_2) + \lambda_3(-2x_3 + 0.25R(x) - u_1y_3(x_3 + 0.125)).\end{aligned}\quad (54)$$

The adjoint advanced ODE (18) becomes

$$\begin{aligned}\dot{\lambda}_1 &= -2x_1 + \lambda_1 + (\lambda_1 - 0.25\lambda_3) \frac{\partial R(x)}{\partial x_1}, \\ \dot{\lambda}_2 &= -2x_2 + \lambda_2 + (\lambda_1 - 0.25\lambda_3) \frac{\partial R(x)}{\partial x_2}, \\ \dot{\lambda}_3 &= -2x_3 + 2\lambda_3 + (\lambda_1 - 0.25\lambda_3) \frac{\partial R(x)}{\partial x_3} + \lambda_3 u_1 y_3 + \chi_{[0, 0.2-r]}(t) \lambda_3^+ u_1^+ (x_3^+ + 0.125),\end{aligned}$$

where  $y_3 = x_3(t-r)$ ,  $x_3^+ = x_3(t+r)$ ,  $u_1^+ = u_1(t+r)$  and  $\lambda_3^+ = \lambda_3(t+r)$ . Since the terminal state  $x(0.2)$  is fixed, no boundary conditions are prescribed for  $\lambda(0.2)$ . The computed

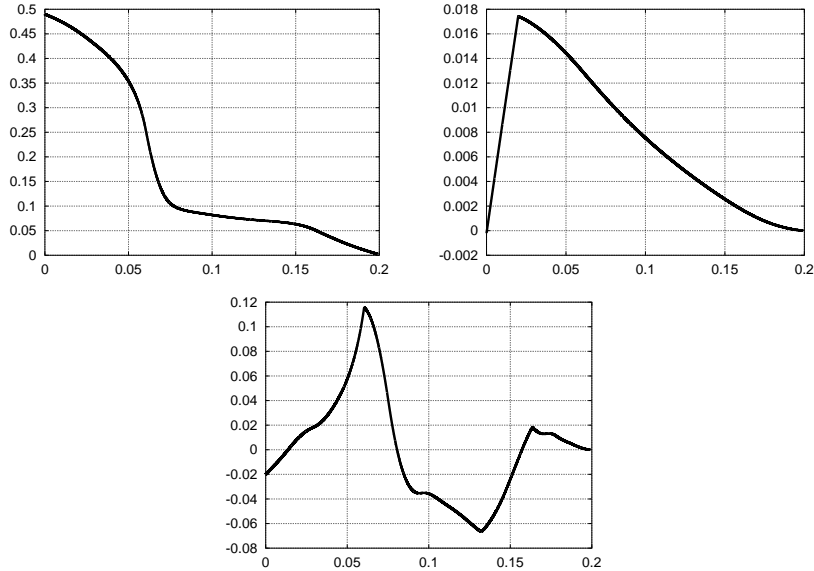


Figure 5: Optimal concentrations  $x_1, x_2$  and optimal temperature  $x_3$

initial value is  $\lambda(0) = (0.048251674, -0.000949667, -0.123610902)$ . The evaluation of the minimum condition (14) is as follows. The control component  $u_1$  appears linearly in the system and is not delayed. Then the switching function (37) is given by

$$\sigma_1(t) = \frac{\partial \mathcal{H}}{\partial u_1}(t) = -\lambda_3(t)x_3(t-r)(x_3(t) + 0.125). \quad (55)$$

*Bang-bang arcs* of  $u_1$  are determined by the control law

$$u_1(t) = \begin{cases} -500, & \text{if } \sigma(t) > 0 \\ +500, & \text{if } \sigma(t) < 0 \end{cases} \quad (56)$$

A *singular arc* of  $u_1$  is characterized by the property that  $\sigma(t) \equiv 0$  holds on a nontrivial subinterval. However, in contrast to undelayed control problems, it is not possible to find a closed expression for a singular control  $u_1$  by differentiating the switching function. Fig. 6 shows that the control  $u_1$  has 6 bang-bang arcs and one intermediate singular arc. We have jointly plotted  $u_1(t)$  and the adequately scaled  $\sigma(t)$  to demonstrate that the behavior of the switching function perfectly matches the control law (56).

As the control component  $u_2$  appears quadratically in the cost functional and is unconstrained, it is determined uniquely by minimum condition (20) which yields

$$\frac{\partial \mathcal{H}}{\partial u_2}(t) + \chi_{[0,0.2]}(t+s) \frac{\partial \mathcal{H}}{\partial u_2}(t+s) = 0 \quad \text{for } t \in [0, 0.2].$$

Thus we have

$$0.02u_2(t) + 0.1\lambda_2(t) + \chi_{[0,0.2]}(t+s) 0.9\lambda_2(t+s) = 0 \quad \text{for } t \in [0, 0.2],$$

which in view of  $0.2 - s = 0.18$  determines the control  $u_2$  by

$$u_2(t) = \begin{cases} -5\lambda_2(t) - \chi_{[0,0.2]}(t+s) \cdot 45\lambda_2(t+s) & \text{for } t \in [0, 0.18] \\ -5\lambda_2(t) & \text{for } t \in [0.18, 0.2] \end{cases}. \quad (57)$$

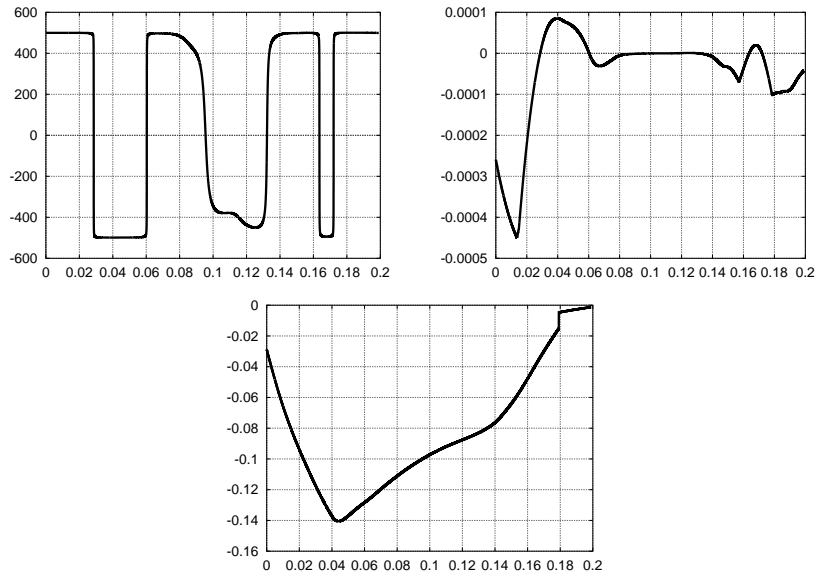


Figure 6: Optimal control function  $u_1$ , switching function  $\sigma_1$  and optimal control  $u_2$ .

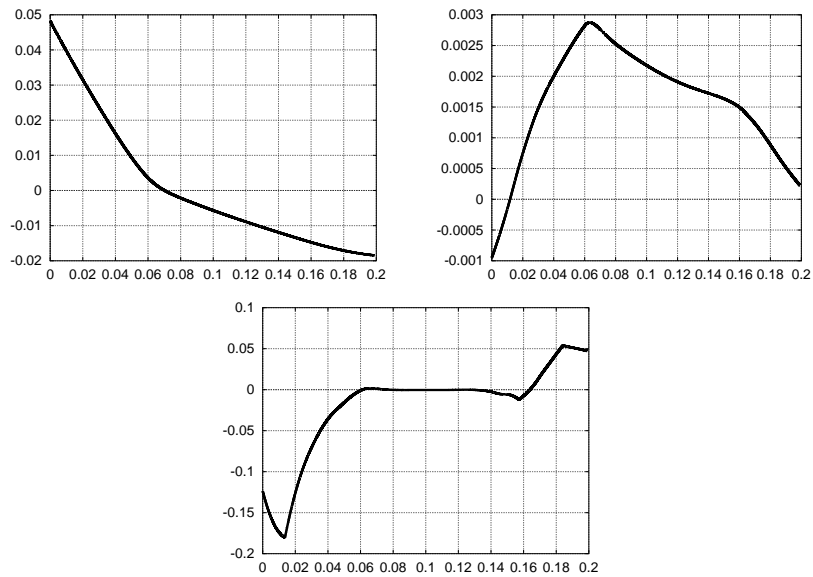


Figure 7: Adjoint variables  $\lambda_1, \lambda_2, \lambda_3$ .

The control law (57) shows that the control  $u_2$  exhibits here a single discontinuity at  $t = 0.18$  provided that  $\lambda_2(0.18) \neq 0$  holds. This behavior is different from the undelayed case where the regularity condition of the Hamiltonian function implies the continuity of control.

**Remark:** The rather large computing time of several hours for this CSTR problem is caused by three factors: (1) the delay in the control variable  $u_2$ , (2) the control  $u_1$  is not penalized in the cost functional, and (3) the prescribed terminal conditions  $x(0.2) = (0, 0, 0)$ . The convergence is speeded up considerably by introducing the penalty term  $0.01u_1(t)^2$  in the cost functional and deleting the terminal conditions. This situation occurs in a similar CSTR problem with  $n = 4$  state variables but no delay in the control variable; cf. Dadebo, Luus [9]. Using a fine grid with  $N = 20000$ , the CPU time for computing the optimal solution of this CSTR problem is in the range of a minute.

## 8 Optimal control of a renewable resource

In this section, we discuss the optimal control of a logistic growth process. Such a model can be used in biology to describe pathogenic cell growth in inflammatory processes, whereas in economy it describes the interaction between production and consumption or the harvesting of a renewable resource.

A well-known example is optimal fishing, where the fact, that overfishing reduces the profit for the fishing industry in the long run, indicates the importance of developing of a long-time fishing strategy.

The following model is based on models developed by May [20, 21] and has been studied by Feddermann [10]. Let  $x(t)$  denote the biomass population and  $u(t)$  the harvesting effort. In the following control model with fixed final time  $t_f > 0$ , only the state variable  $x(t)$  has a delay  $r \geq 0$ :

$$\text{Maximize } J(u, x) = \int_0^{t_f} e^{-dt} (pu(t) - c_E x(t)^{-1} u(t)^3) dt \quad (58)$$

subject to

$$\dot{x}(t) = ax(t) \left( 1 - \frac{x(t-r)}{b} \right) - u(t), \quad (59)$$

$$x(t) \equiv x_0, \quad t \in [-r, 0], \quad (60)$$

$$x(t) \geq x_0, \quad t \in [0, t_f], \quad (61)$$

$$u(t) \geq 0, \quad t \in [0, t_f]. \quad (62)$$

A similar model with a linear cost functional was considered in Clarke, Wolenski [7] as an illustrative example to compute the sensitivity of the value function with respect to the time-lag  $r$ . The data are chosen as follows: market price  $p = 2$ , discount rate  $d = 0.05$ , harvesting cost  $c_E = 0.2$ , growth rates  $a = 3$  and  $b = 5$ , initial value  $x_0 = 2$  and final time  $t_f = 20$ .

For these data, our computations show the state and control inequality constraints (61) and (62) do not become active. Hence, we do need to take into account the multiplier  $\mu$

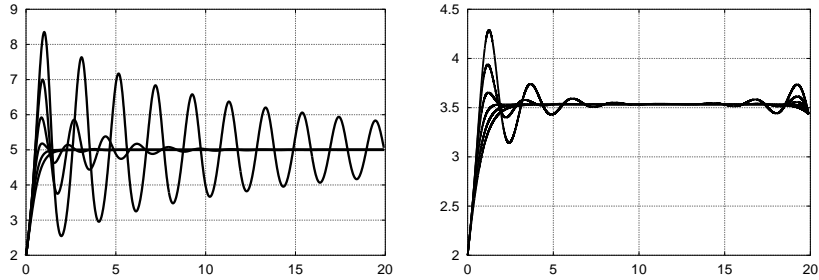


Figure 8: Delays  $r = 0, 0.1, 0.2, 0.3, 0.4, 0.5$  (bottom-up): (a) uncontrolled state trajectories  $x(t)$ , (b) optimal state trajectories  $x(t)$ .

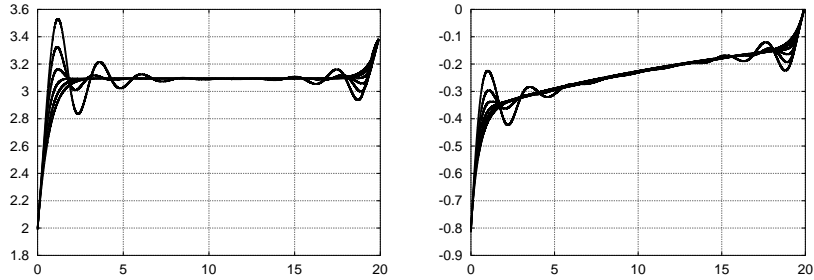


Figure 9: Delays  $r = 0, 0.1, 0.2, 0.3, 0.4, 0.5$  (bottom-up): (a) optimal control  $u(t)$  and (b) adjoint variable  $\lambda(t)$ .

in the Hamiltonian (7) which is given here by (note that we are minimizing):

$$\mathcal{H}(t, x, y, u, \lambda) = e^{-dt}(-pu + c_E x^{-1} u^3) + \lambda \left( ax \left( 1 - \frac{y}{b} \right) - u \right).$$

The adjoint equation (18) and transversality condition (19) yield

$$\begin{aligned} \dot{\lambda}(t) &= c_E e^{-dt} x^{-2}(t) u^3(t) - a \lambda(t) \left( 1 - \frac{x(t-r)}{b} \right) \\ &+ \chi_{[0, t_f]}(t+r) \lambda(t+r) \frac{a}{b} x(t+r), \quad \lambda(t_f) = 0. \end{aligned} \quad (63)$$

The minimum condition (20) implies

$$0 = \frac{\partial \mathcal{H}}{\partial u}(t) = e^{-dt}(-p + 3c_E x^{-1}(t) u^2(t)) - \lambda(t),$$

which gives the control relation using the above data:

$$u(t) = \sqrt{\frac{5}{3} \exp(0.05t) x(t) \lambda(t) + \frac{10}{3} x(t)}. \quad (64)$$

We apply the discretization methods in section 5 and solve the resulting nonlinear programming problem (NLP) with a mesh size of  $N = 40000$  grid points by the Interior Point Code LOQO developed by Vanderbei [31, 32]. For different delays  $r \geq 0$ , the uncontrolled state trajectories  $x(t)$  with  $u(t) = 0$  are shown in Fig. 8(a) and are contrasted in Fig. 8(b) with the *optimal* state trajectories. Optimal controls and the associated adjoint functions are depicted in Fig. 9. Feddermann [10] has obtained similar results using the optimal control package NUDOCSS developed by Büskens [4]. We conclude this section by listing the computed values of the (maximized) objective functional (58) and the initial values  $\lambda(0)$  for different delays:

$$\begin{aligned}
r = 0.0 : & \quad J = 56.290449, \quad \lambda(0) = -0.797255 \\
r = 0.1 : & \quad J = 56.416287, \quad \lambda(0) = -0.801229 \\
r = 0.2 : & \quad J = 56.542214, \quad \lambda(0) = -0.805113 \\
r = 0.3 : & \quad J = 56.662908, \quad \lambda(0) = -0.808916 \\
r = 0.4 : & \quad J = 56.780054, \quad \lambda(0) = -0.812444 \\
r = 0.5 : & \quad J = 56.876896, \quad \lambda(0) = -0.815298
\end{aligned}$$

Clarke, Wolenski [7] have presented conditions under which the optimal value function  $V = V(r)$  is differentiable w.r.t. the delay  $r$ . It would be of interest to verify their explicit formula numerically for the derivative  $dV/dr$  of the value function at  $r = 0$ . The above results yield the crude approximation  $dV(r)/dr \approx 1.2$  at  $r = 0$ .

## 9 Conclusion

The purpose of this paper was twofold. Firstly, a Pontryagin type minimum principle was derived for retarded optimal control problems with delays in the state and control variable when the control system is subject to a mixed control-state constraint. Under the assumption that the ratio of state and control delay is a rational number (this is not a restriction for numerical computation), the retarded control system was transformed to an augmented nondelayed control problem, to which the classical Pontryagin minimum principle is applicable. Then a suitable retransformation of state, control and adjoint variables yields the minimum principle for the retarded control problem. The second goal was to develop efficient numerical methods for computing the optimal state, control and adjoint variables. In particular, the adjoint variables enable us to check the the necessary optimality conditions with high accuracy. We have presented a discretization method (for simplicity only Euler's method) whereby the control problem is transcribed into a high-dimensional nonlinear programming problem. Excellent results have been obtained using the optimization solvers LOQO by Vanderbei [31], IPOPT by Wächter et al. [33, 34] or, alternatively, the solver NUDOCSS by Büskens [4].

Several issues for retarded control problems, which could not adequately be addressed in this paper, require further work. The theory of bang–bang and singular control problems initiated by Soliman, Ray [30] should be studied in more detail; cf. also Kern [19]. The transformation techniques in section 4 can also be applied to retarded control problems with *pure* state inequality constraints. This approach will eventually lead to conditions, under which the multipliers associated with state constraints (cf. Angell, Kirsch [1]) are sufficiently regular. Finally, the theory of second order sufficient conditions (cf. Chan, Yung [6] for unconstrained control problems) should be generalized to control problems with constraints and must be made amenable to numerical verification.

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