

Optimal time delays in a class of reaction-diffusion equations

E. Casas^a, M. Mateos^b and F. Tröltzsch^c

^aDepartamento de Matemática Aplicada y Ciencias de la Computación, E.T.S.I. Industriales y de Telecomunicación, Universidad de Cantabria, 39005 Santander, Spain; ^bDepartamento de Matemáticas, Campus de Gijón, Universidad de Oviedo, 33203, Gijón, Spain; ^cInstitut für Mathematik, Technische Universität Berlin, D-10623 Berlin

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ABSTRACT

A class of semilinear parabolic reaction diffusion equations with multiple time delays is considered. These time delays and corresponding weights are to be optimized such that the associated solution of the delay equation is the best approximation of a desired state function. The differentiability of the mapping is proved that associates the solution of the delay equation to the vector of weights and delays. Based on an adjoint calculus, first-order necessary optimality conditions are derived. Numerical test examples show the applicability of the concept of optimizing time delays.

KEYWORDS

semilinear parabolic equation, multiple time delays, Pyragas type feedback, optimization, learning controller

AMS CLASSIFICATION

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1. Introduction

In this paper, we consider the optimization of Pyragas type feedback controllers in reaction-diffusion equations with respect to finitely many time delays. The simplest example of an associated optimization problem is the following: Let the semilinear parabolic equation with time delay $s \geq 0$

$$\frac{\partial}{\partial t}y(x, t) - \Delta y(x, t) + R(y(x, t)) = \kappa(y(x, t - s) - y(x, t)), \quad (x, t) \in Q \quad (1)$$

be given in $Q := \Omega \times (0, T)$, where $\Omega \subset \mathbb{R}^d$, $d \leq 3$, is a bounded Lipschitz domain. The equation is complemented by homogeneous Neumann boundary conditions and associated initial conditions.

Email: eduardo.casas@unican.es

Email: mmateos@uniovi.es

CONTACT Email: troeltzsch@math.tu-berlin.de

Find a time delay s and a weight $\kappa \in \mathbb{R}$ such that the associated state function y minimizes the distance to a desired state function y_Q in the norm of $L^2(Q)$. In particular, we directly optimize, say "control", the time delay s .

The optimization with respect to finitely many time delays and weights, associated first-order necessary optimality conditions, and numerical tests constitute the main novelty of our paper.

In view of the needed differentiability of the mapping $s \mapsto y$, the theory of optimality conditions turns out to be quite delicate. This differentiability issue was investigated first by Hale and Ladeira in [1] for ordinary differential equations and in [2] for non-linear reaction-diffusion equations. They proved a version that is local in time, since under their assumptions the solution y could blow up in finite time. By a different method including certain monotonicity arguments, we were able to prove a general result on existence and uniqueness for nonlocal reaction-diffusion equations including measures in [3]. This result is valid for arbitrary time horizons $T > 0$ and includes the equations considered here. Having this at our disposal, the proof of differentiability with respect to time delays became possible for arbitrary $T > 0$.

More generally, we will consider multiple time delays s_i and associated weights κ_i , $i = 1, \dots, m$, cf. equation (2) below. To our best knowledge, the optimization with respect to time delays s_i and associated weights κ_i was not yet investigated in literature. Compared with optimal control problems, the time delay s and the weight κ play the role of the control, while y is the state function of the control system. Although $u = (s, \kappa)$ is not a control in the standard sense, we will occasionally call this vector a control.

This question might be interesting for applications. For instance, in laser technology, feedback controllers of Pyragas type are considered. Here, a laser beam is partially reflected by a semi-permeable mirror and the reflected part is fed back after some time delay s . More general, a finite number of mirrors can be used giving rise to finitely many time delays s_1, \dots, s_m . Then, instead of (1), the more general equation

$$\frac{\partial}{\partial t} y(x, t) - \Delta y(x, t) + R(y(x, t)) = \sum_{i=1}^m \kappa_i y(x, t - s_i) \quad (2)$$

is of interest, where the vectors $s = (s_1, \dots, s_m)$ and $\kappa = (\kappa_1, \dots, \kappa_m)$ are at our disposal. For Pyragas type problems with single or multiple time delays, the reader is referred to [4,5], the survey volume [6], and exemplarily to the papers [7–9].

Our optimization problems with respect to the equation (2) are somehow intermediate between the ones in our former contributions [10] and [3] that investigate the optimization of feedback kernels in nonlocal reaction-diffusion equations. In [10], a nonlocal Pyragas type control system of the form

$$\frac{\partial}{\partial t} y(x, t) - \Delta y(x, t) + R(y(x, t)) = \kappa \left[\int_0^T g(s) y(x, t - s) ds - y(x, t) \right] \quad (3)$$

is considered, where the kernel function g is to be optimized, i.e. it plays the role of a control. Later, in [3], we allowed measures as controls so that, in particular, Dirac measures could appear,

$$\frac{\partial}{\partial t} y(x, t) - \Delta y(x, t) + R(y(x, t)) = \int_0^T y(x, t - s) d\mu(s), \quad (4)$$

where the control μ is a regular Borel measure on $[0, T]$.

Our control system cannot be subsumed as a particular case of (4). In (4), the measure μ can be composed of an absolutely continuous part (that is somehow related to g in (3)) and a singular part that can be a combination of Dirac measures. There is no a priori information on how the structure is, how many Dirac measures appear, and where they are concentrated. In this sense, (4) is much more general than (2). On the other hand, the optimization of (2) is restricted to a subset of the admissible controls for (4); in (2) the measure μ is required to be a linear combination of m Dirac measures δ_{s_i} , $i \in \{1, \dots, m\}$, with m fixed.

This restriction to finitely many Dirac measures might be dictated by the technical background. In the application to Laser technology mentioned above, the number of semi-permeable mirrors might be fixed for a given construction. Another application comes from medical science. For instance, in Holt and Netoff [11], linear combinations of a fixed number of Dirac measures are used in experiments that are related to the treatment of Parkinson's disease.

Our paper is organized as follows: In Section 2, we define and analyze our optimization problem. First, we prove the differentiability of the mapping $s \mapsto y_s$. In principle, this differentiability is known from [2]. However, in the setting of [2], the existence of y is only known locally in an interval $[0, \alpha)$. At α , the solution y can blow up. A new version of the Banach fixed-point theorem was applied to prove differentiability. In our case, thanks to certain monotonicity properties, we have global existence on any interval $[0, T]$ and are able to prove differentiability of the control-to-state mapping. Then, the existence of a solution and the optimality conditions is addressed. Section 3 is devoted to the numerical discretization of the problem. In Section 4 we present some numerical examples that show the applicability of our concept of controlling time delays.

2. Analysis of the optimization problem

In this work, Ω is a domain of \mathbb{R}^d , $d \leq 3$, with Lipschitz boundary Γ , while $T > 0$ is a fixed final time; we will write $Q = \Omega \times (0, T)$ and $\Sigma = \Gamma \times (0, T)$. Moreover, we fix $m \in \mathbb{N}$, real parameters $0 \leq a_i \leq b_i$, $i = 1, \dots, m$, and set $b = \max\{b_i : i = 1, \dots, m\}$ and $Q^- = \Omega \times (-b, 0)$. We assume that $b < T$.

The initial data are defined in \bar{Q}^- by a continuous function $y_0 : \bar{Q}^- \rightarrow \mathbb{R}$. The reaction term is given by a function $R : Q \times \mathbb{R} \rightarrow \mathbb{R}$. The assumptions on Ω , y_0 , and R will be detailed later.

Finally, we introduce the admissible set

$$U_{ad} = \{u = (s, \kappa) \in \mathbb{R}^m \times \mathbb{R}^m : a_i \leq s_i \leq b_i, \alpha_i \leq \kappa_i \leq \beta_i, 1 \leq i \leq m\},$$

where $-\infty \leq \alpha_i \leq \beta_i \leq \infty$, $i = 1, \dots, m$, are given real numbers.

We consider the optimization problem

$$(P) \quad \min_{u \in U_{ad}} J(u) = \frac{1}{2} \int_Q (y_u - y_Q)^2 dxdt + \frac{\nu}{2} |\kappa|^2,$$

where $\nu \geq 0$, $|\kappa|$ denotes the Euclidean norm of κ in \mathbb{R}^m , and y_u is the unique solution

of the state equation (5) below,

$$\left\{ \begin{array}{ll} \partial_t y - \Delta y + R(x, t, y) = \sum_{i=1}^m \kappa_i y(x, t - s_i) & \text{in } Q \\ \partial_n y = 0 & \text{on } \Sigma \\ y(x, t) = y_0(x, t) & \text{in } Q^-. \end{array} \right. \quad (5)$$

By ∂_n , we denote the outward normal derivative on Γ .

Notice that the right hand side of (5) can be written as

$$\sum_{i=1}^m \kappa_i y(x, t - s_i) = \int_{[0, T]} y(x, t - s) d\mu(s)$$

with $\mu = \sum_{i=1}^m \kappa_i \delta_{s_i} \in \mathcal{M}[0, T]$.

Let us mention that the right-hand side of (5) is more general than a standard Pyragas feedback as in equation (1) that includes the term $-y(x, t)$ in the right-hand side. This term is obtained in (5) by the particular delay $s_1 = 0$ with a suitable coefficient.

We impose the following assumptions on the given data in (P).

- (A1) The domain Ω is $W^{2,q}$ regular for some $q > \frac{d}{2} + 1$, i.e., if $y \in H^1(\Omega)$, $\Delta y \in L^q(\Omega)$ and $\partial_n y \in W^{1-1/q, q}(\Gamma)$, then $y \in W^{2,q}(\Omega)$.
- (A2) We require $y_0 \in C(\bar{Q}^-) \cap W^{1,q}(-b, 0; L^q(\Omega))$ and $y_0(\cdot, 0) \in W^{2-\frac{2}{q}, q}(\Omega)$.
- (A3) R is a Carathéodory function of class C^1 with respect to the last variable such that

$$\begin{aligned} R(\cdot, \cdot, 0) &\in L^q(Q), \\ \exists C_R \in \mathbb{R} : \partial_y R(x, t, y) &\geq C_R, \quad \forall y \in \mathbb{R}, \\ \forall M > 0 \exists C_M : |\partial_y R(x, t, y)| &\leq C_M, \quad \forall |y| \leq M, \end{aligned}$$

holds for almost all $(x, t) \in Q$.

Notice that (A1) is satisfied in convex plane polygonal domains or in domains with boundary of class $C^{1,1}$.

We will consider the state space

$$\mathcal{Y} = C(\bar{Q}) \cap W_q^{2,1}(Q),$$

where $W_q^{2,1}(Q) = L^q(0, T; W^{2,q}(\Omega)) \cap W^{1,q}(0, T; L^q(\Omega))$; \mathcal{Y} is a Banach space endowed with the usual intersection norm.

Theorem 2.1. *Under assumptions (A1), (A2), and (A3), for every $u \in U_{ad}$ there exists a unique solution $y_u \in \mathcal{Y}$ of (5). Moreover, for all $r > 0$ there exists a constant C_r such that*

$$\|y_u\|_{\mathcal{Y}} \leq C_r \left(\|y_0\|_{C(\bar{Q}^-)} \sum_{i=1}^m |\kappa_i| + \|y_0(\cdot, 0)\|_{W^{2-\frac{2}{q}, q}(\Omega)} + \|R(\cdot, \cdot, 0)\|_{L^q(Q)} \right)$$

holds for all $u = (s, \kappa) \in \mathbb{R}^m \times \mathbb{R}^m$ with $|\kappa| \leq r$.

Proof. Existence and uniqueness of the solution $y_u \in C(\bar{Q}) \cap L^2(0, T; H^1(\Omega))$ follow from [3, Th. 2.2] with $u = \sum_{i=1}^m \kappa_i \delta_{s_i}$, where the following estimate is proved

$$\|y_u\|_{C(\bar{Q})} \leq c_r \left(\|y_0\|_{C(\bar{Q}^-)} \|u\|_{\mathcal{M}[0, T]} + \|y_0(\cdot, 0)\|_{C(\bar{\Omega})} + \|R(\cdot, \cdot, 0)\|_{L^q(Q)} \right).$$

Notice that $\|u\|_{\mathcal{M}[0, T]} = \sum_{i=1}^m |\kappa_i|$. Once this is obtained, from (5) and assumptions (A1)-(A3) we infer $\partial_t y_u - \Delta y_u \in L^q(Q)$. Now, the $W_q^{2,1}(Q)$ regularity and the corresponding estimate follows from [12, Th. IV.9.1] and the inequality established above. \square

We mention that the function \tilde{y}_u , defined by

$$\tilde{y}_u(x, t) = \begin{cases} y_u(x, t), & 0 \leq t \leq T, \\ y_0(x, t), & -b \leq t < 0, \end{cases}$$

belongs to $W^{1,q}(-b, T; L^q(\Omega))$. This is a consequence of the regularity established in the theorem and assumption (A2). In what follows, when this does not lead to confusion, we will identify y_u with its extension \tilde{y}_u .

By the next result, we improve the differentiability result of [2].

Theorem 2.2. *The control-to-state mapping $G : U_{ad} \rightarrow \mathcal{Y}$, $u \mapsto y_u$ has partial derivatives $\partial_{s_i} G(u)$ and $\partial_{\kappa_i} G(u)$ given as follows: For every $u \in U_{ad}$ and $1 \leq i \leq m$, we have $\partial_{s_i} G(u) = z_i$ where z_i satisfies the equation*

$$\begin{cases} \partial_t z - \Delta z + \partial_y R(x, t, y_u) z = \sum_{j=1}^m \kappa_j z(x, t - s_j) - \kappa_i \partial_t y_u(x, t - s_i) & \text{in } Q \\ \partial_n z = 0 & \text{on } \Sigma, \quad z = 0 & \text{in } Q^-, \end{cases} \quad (6)$$

and $\partial_{\kappa_i} G(u) = \eta_i$, where η_i satisfies

$$\begin{cases} \partial_t \eta - \Delta \eta + \partial_y R(x, t, y_u) \eta = \sum_{j=1}^m \kappa_j \eta(x, t - s_j) + y_u(x, t - s_i) & \text{in } Q \\ \partial_n \eta = 0 & \text{on } \Sigma, \quad \eta = 0 & \text{in } Q^-. \end{cases} \quad (7)$$

Proof. We fix $u = (s, \kappa) \in U_{ad}$ and write $y = G(u) = G(s, \kappa)$. First, we calculate the partial derivative with respect to s_i . For sufficiently small $|\rho|$, we write $y_\rho = G(s + \rho e_i, \kappa)$, where e_i denotes the i -th vector of the canonical base of \mathbb{R}^m . We have to compute

$$\partial_{s_i} G(s, \kappa) = \lim_{\rho \rightarrow 0} \frac{y_\rho - y}{\rho},$$

where the limit is restricted to $\rho > 0$ if $s_i = a_i$ and to $\rho < 0$ if $s_i = b_i$, since we have to determine the right and left derivatives in these points, respectively. Define $z_\rho = \frac{y_\rho - y}{\rho}$; subtracting the partial differential equations and dividing by ρ we get by the mean

value theorem for $\hat{y}_\rho(x, t) = y(x, t) + \theta(x, t)(y_\rho(x, t) - y(x, t))$, $0 < \theta(x, t) < 1$,

$$\begin{aligned} & \partial_t z_\rho - \Delta z_\rho + \partial_y R(x, t, \hat{y}_\rho) z_\rho \\ &= \sum_{j \neq i} \kappa_j \frac{y_\rho(x, t - s_j) - y(x, t - s_j)}{\rho} + \kappa_i \frac{y_\rho(x, t - s_i - \rho) - y(x, t - s_i)}{\rho} \\ &= \sum_{j \neq i} \kappa_j z_\rho(x, t - s_j) + \kappa_i z_\rho(x, t - s_i - \rho) + \kappa_i \frac{y(x, t - s_i - \rho) - y(x, t - s_i)}{\rho}. \end{aligned} \quad (8)$$

Using Theorem 2.1 and taking into account that $z(0) = 0$ in Ω and $\partial_n z = 0$ on Σ , we deduce

$$\begin{aligned} \|z_\rho\|_{\mathcal{Y}} &\leq C \left(\int_Q \left(\frac{y(x, t - s_i - \rho) - y(x, t - s_i)}{\rho} \right)^q dx dt \right)^{1/q} \\ &= C \left\| \frac{y(\cdot, \cdot - s_i - \rho) - y(\cdot, \cdot - s_i)}{\rho} \right\|_{L^q(Q)} \end{aligned} \quad (9)$$

with some constant $C > 0$, which may depend on κ , but is independent of ρ and s . Since $y \in W^{1,q}(0, T, L^q(\Omega))$, we have that

$$\lim_{\rho \rightarrow 0} \frac{y(x, t - s_i - \rho) - y(x, t - s_i)}{\rho} = -\partial_t y(x, t - s_i) \text{ in } L^q(Q). \quad (10)$$

Indeed, consider $\varepsilon > 0$ arbitrary. Then, for all $|\rho|$ small enough, applying [13, Thm 1.1 in page 57], we obtain

$$\begin{aligned} & \left(\int_Q \left(\frac{y(x, t - s_i - \rho) - y(x, t - s_i)}{\rho} + \partial_t y(x, t - s_i) \right)^q dx dt \right)^{1/q} \\ &= \left(\int_Q \left(- \int_0^1 (\partial_t y(x, t - s_i - \lambda\rho) - \partial_t y(x, t - s_i)) d\lambda \right)^q dx dt \right)^{1/q} \\ &= \left\| - \int_0^1 (\partial_t y(\cdot, \cdot - s_i - \lambda\rho) - \partial_t y(\cdot, \cdot - s_i)) d\lambda \right\|_{L^q(Q)} \\ &\leq \int_0^1 \|\partial_t y(\cdot, \cdot - s_i - \lambda\rho) - \partial_t y(\cdot, \cdot - s_i)\|_{L^q(Q)} d\lambda \\ &< \int_0^1 \varepsilon d\lambda = \varepsilon. \end{aligned}$$

From (9) and (10), we deduce that $\{z_\rho\}_\rho$ is uniformly bounded in \mathcal{Y} . Hence we can extract a subsequence that converges weakly in \mathcal{Y} to some z . Since \mathcal{Y} is compactly embedded in $L^q(Q)$, we also have that $z_\rho \rightarrow z$ strongly in $L^q(Q)$. Since the right hand side of (8) is bounded in $L^q(Q)$ and $y_0(\cdot, 0)$ is a Hölder function in $\bar{\Omega}$, we have that there exists $\mu \in (0, 1)$ such that $\{z_\rho\}_\rho$ is bounded in $C^{0,\mu}(\bar{Q})$, see [12, III-10]. Using that $C^{0,\mu}(\bar{Q})$ is compactly embedded in $C(\bar{Q})$, we have that $z_\rho \rightarrow z$ strongly in $C(\bar{Q})$. Passing to the limit in (8), in view of (10), we obtain (6).

Now, we calculate the partial derivative with respect to κ_i . For small $|\rho|$, we define $y_\rho = G(s, \kappa + \rho e_i)$ and $\eta_\rho = (y_\rho - y)/\rho$. As above, there exists $\hat{y}_\rho(x, t) = y(x, t) + \theta(x, t)(y_\rho(x, t) - y(x, t))$ with some measurable function $0 < \theta(x, t) < 1$ such that

$$\partial_t \eta_\rho - \Delta \eta_\rho + \partial_y R(x, t, \hat{y}_\rho) \eta_\rho = \sum_{j=1}^m \kappa_j \eta_\rho(x, t - s_j) + y_\rho(x, t - s_i).$$

Again $\{\eta_\rho\}_\rho$ is uniformly bounded in $\mathcal{Y} \cap C^{0,\mu}(\bar{Q})$ for some $\mu > 0$, and we can pass to the limit to obtain (7). \square

By Theorem 2.2 and the chain rule, the functional J is differentiable and its derivative has the following form.

Theorem 2.3. *The functional J has partial derivatives*

$$\frac{\partial J}{\partial s_i}(u) = -\kappa_i \int_Q \varphi_u(x, t) \partial_t y_u(x, t - s_i) dx dt, \quad (11)$$

$$\frac{\partial J}{\partial \kappa_i}(u) = \nu \kappa_i + \int_Q \varphi_u(x, t) y_u(x, t - s_i) dx dt, \quad (12)$$

for $1 \leq i \leq m$, where the adjoint state $\varphi_u \in \mathcal{Y}$ is the unique solution to the advanced adjoint equation

$$\begin{cases} -\partial_t \varphi - \Delta \varphi + \partial_y R(x, t, y_u) \varphi = y_u - y_Q + \sum_{i=1}^m \kappa_i \varphi(x, t + s_i) & \text{in } Q \\ \partial_n \varphi(x, t) = 0 & \text{on } \Sigma, \varphi(x, t) = 0 & \text{if } t \geq T. \end{cases} \quad (13)$$

Proof. Using the chain rule, we obtain

$$\frac{\partial J}{\partial s_i}(u) = \int_Q (y_u - y_Q) z_i dx dt \quad \text{and} \quad \frac{\partial J}{\partial \kappa_i}(u) = \int_Q (y_u - y_Q) \eta_i dx dt + \nu \kappa_i,$$

where $z_i \in \mathcal{Y}$ is the solution of (6) and η_i is the solution of (7).

Let us consider the derivative with respect to s_i . Using the adjoint state equation (13), integration by parts and the equation (6) satisfied by z_i , we obtain

$$\begin{aligned} \int_Q (y_u - y_Q) z_i dx dt &= \\ &= \int_Q \left[-\partial_t \varphi_u - \Delta \varphi_u + \partial_y R(x, t, y_u) \varphi_u - \sum_{j=1}^m \kappa_j \varphi_u(x, t + s_j) \right] z_i dx dt \\ &= \int_Q \varphi_u \left[\partial_t z_i - \Delta z_i + \partial_y R(x, t, y_u) z_i - \sum_{j=1}^m \kappa_j z_i(x, t - s_j) \right] dx dt \\ &= -\kappa_i \int_Q \varphi_u(x, t) \partial_t y_u(x, t - s_i) dx dt. \end{aligned}$$

Here we performed the change of variables $\tilde{t} = t + s_j$ and took into account the final conditions satisfied by φ_u along with the initial conditions satisfied by z_i to write

$$\int_Q \varphi_u(x, t + s_j) z_i(x, t) dt dx = \int_Q \varphi_u(x, t) z_i(x, t - s_j) dt dx$$

The derivative with respect to κ_i is obtained in a similar way. \square

Next, we show the well-posedness of (P).

Theorem 2.4. *If $\nu > 0$ or $-\infty < \alpha_i \leq \beta_i < \infty$ for all $i \in \{1, \dots, m\}$, then Problem (P) has a solution $\bar{u} = (\bar{s}, \bar{\kappa})$.*

Proof. If $u^k = (s^k, \kappa^k) \rightarrow u = (s, \kappa)$ in $\mathbb{R}^m \times \mathbb{R}^m$, then $\sum_{i=1}^m \kappa_i^k \delta_{s_i^k} \xrightarrow{*} \sum_{i=1}^m \kappa_i \delta_{s_i}$ in $\mathcal{M}[0, T]$ as $k \rightarrow \infty$. So following [3, Lemma 3.2], we have that $y_{u^k} \rightarrow y_u$ strongly in $L^2(0, T; H^1(\Omega)) \cap C(\bar{Q})$. Therefore J is continuous in U_{ad} and obviously U_{ad} is closed in $\mathbb{R}^m \times \mathbb{R}^m$.

Thanks to our assumptions, either the objective functional is coercive or U_{ad} is compact. Since we are dealing with a finite dimensional problem, it is clear that (P) has a global solution. \square

Now we are able to set up the first order necessary optimality conditions.

Theorem 2.5. *Let $\bar{u} \in U_{ad}$ be a local solution of (P) and let \bar{y} be the associated state defined by*

$$\begin{cases} \partial_t \bar{y} - \Delta \bar{y} + R(\bar{y}) = \sum_{j=1}^m \bar{\kappa}_j \bar{y}(x, t - \bar{s}_j) & \text{in } Q \\ \partial_n \bar{y} = 0 & \text{on } \Sigma \\ \bar{y}(x, t) = y_0(x, t) & \text{in } Q^- \end{cases} \quad (14)$$

Then there exists a unique adjoint state $\bar{\varphi} \in \mathcal{Y}$ such that the adjoint equation

$$\begin{cases} -\partial_t \bar{\varphi} - \Delta \bar{\varphi} + \partial_y R(x, t, \bar{y}) \bar{\varphi} = \bar{y} - y_0 + \sum_{i=1}^m \bar{\kappa}_i \bar{\varphi}(x, t + \bar{s}_i) & \text{in } Q \\ \partial_n \bar{\varphi} = 0 & \text{on } \Sigma \\ \bar{\varphi} = 0 & \text{if } t \geq T, \end{cases} \quad (15)$$

the variational inequalities

$$-\bar{\kappa}_i \int_Q \partial_t \bar{y}(x, t - \bar{s}_i) \bar{\varphi}(x, t) dx dt (s_i - \bar{s}_i) \geq 0 \quad \forall s_i \in [a_i, b_i], \quad (16)$$

and

$$\left(\nu \bar{\kappa}_i + \int_Q \bar{y}(x, t - \bar{s}_i) \bar{\varphi}(x, t) dx dt \right) (\kappa_i - \bar{\kappa}_i) \geq 0 \quad \forall \kappa_i \in [\alpha_i, \beta_i] \cap \mathbb{R}, \quad (17)$$

are satisfied for $i = 1, \dots, m$.

3. Numerical Discretization

We suppose that Ω is polygonal or polyhedral and consider, cf. [14, definition (4.4.13)], a quasi-uniform family of triangulations $\{\mathcal{K}_h\}_{h>0}$ of $\bar{\Omega}$ and a quasi-uniform family of partitions of size τ of $[0, T]$, $0 = t_0 < t_1 < \dots < t_{N_\tau} = T$. We define $I_k = (t_{k-1}, t_k]$, $\tau_k = t_k - t_{k-1}$, $\tau = \max\{\tau_k\}$, and introduce the space-time mesh size $\sigma = (h, \tau)$.

Now we consider the finite dimensional spaces

$$\begin{aligned} Y_h &= \{z_h \in C(\bar{\Omega}) : z_h|_K \in \mathcal{P}^1(K) \ \forall K \in \mathcal{K}_h\}, \\ \mathcal{Y}_\sigma^0 &= \{\phi_\sigma \in L^2(0, T; Y_h) : \phi_\sigma|_{I_k} \in \mathcal{P}^0(I_k; Y_h) \ \forall k = 1, \dots, N_\tau\}, \\ \mathcal{Y}_\sigma^1 &= \{y_\sigma \in C([0, T]; Y_h) : y_\sigma|_{I_k} \in \mathcal{P}^1(I_k; Y_h) \ \forall k = 1, \dots, N_\tau\} \end{aligned}$$

where $\mathcal{P}^1(K)$ is the set of polynomials of degree 1 in K and, for $i = 0, 1$, $\mathcal{P}^i(I_k; Y_h)$ is the set of polynomials of degree i defined in I_k with values in Y_h .

For $\phi_\sigma \in \mathcal{Y}_\sigma^0$, we denote by $\phi_\sigma^k \in Y_h$ the value of ϕ_σ in I_k . We also remark that \mathcal{Y}_σ^1 is contained in $W^{1,q}(0, T; L^q(\Omega))$ and, if $y_\sigma \in \mathcal{Y}_\sigma^1$, then $\partial_t y_\sigma$ can be identified with an element of \mathcal{Y}_σ^0 .

The discrete state equation is defined in a variational form as follows: For given control vector $u = (s, \kappa)$, the associated discrete state $y_\sigma(u) \in \mathcal{Y}_\sigma^1$ is the unique solution of (cf. [15, Eq. (23)])

$$\begin{aligned} y_\sigma(x, 0) &= \Pi_h y_0(x, 0), \\ \int_Q \frac{\partial y_\sigma}{\partial t} \phi_\sigma \, dxdt + \int_Q \nabla_x y_\sigma \nabla_x \phi_\sigma \, dxdt + \int_Q R(x, t, y_\sigma) \phi_\sigma \, dxdt \\ &= \sum_{i=1}^m \kappa_i \left[\int_0^{s_i} y_0(x, t - s_i) \phi_\sigma \, dxdt + \int_{s_i}^T y_\sigma(x, t - s_i) \phi_\sigma \, dxdt \right], \quad \forall \phi_\sigma \in \mathcal{Y}_\sigma^0, \end{aligned} \tag{18}$$

where $\Pi_h : L^2(\Omega) \rightarrow Y_h$ is the projection onto Y_h in the $L^2(\Omega)$ -sense.

The discretized optimization problem is

$$(P_\sigma) \quad \min_{u \in U_{ad}} J_\sigma(u) = \frac{1}{2} \int_Q (y_\sigma(u)(x, t) - y_Q(x, t))^2 \, dxdt + \frac{\nu}{2} |\kappa|^2.$$

To compute the partial derivatives of J_σ , we invoke an associated discrete adjoint equation. For every $u \in U_{ad}$, we define the associated discrete adjoint state $\varphi_\sigma(u) \in \mathcal{Y}_\sigma^0$ as the unique solution of (cf. [15, Eq. (25)])

$$\begin{aligned} \varphi_\sigma^{N_\tau+1} &= 0 \\ &- \sum_{k=1}^{N_\tau} \int_\Omega z_\sigma(x, t_k) (\varphi_\sigma^{k+1} - \varphi_\sigma^k) \, dx + \int_Q \nabla_x z_\sigma \nabla_x \varphi_\sigma \, dxdt \\ &+ \int_Q \partial_y R(x, t, y_\sigma(u)) z_\sigma \varphi_\sigma \, dxdt = \int_Q (y_\sigma(u) - y_Q) z_\sigma \, dxdt \\ &+ \sum_{i=1}^m \kappa_i \int_0^{T-s_i} \int_\Omega \varphi_\sigma(x, t + s_i) z_\sigma \, dxdt, \quad \forall z_\sigma \in \mathcal{Y}_\sigma^1, \end{aligned} \tag{19}$$

where we have introduced an artificial $\varphi_\sigma^{N_\tau+1}$ to simplify the notation.

Both the discrete state equation (18) and the discrete adjoint state equation (19) can be solved using a time-marching scheme. Despite the differences in the variational formulations, in both cases a Crank-Nicholson time-marching scheme is obtained, cf. [15, p. 824].

Remark 1. Notice that the time instants t_k , $k = 1, \dots, N_\tau$, can be taken completely independent of the location of the time delays. Moreover, the time delays can admit any value between 0 and b ; they also can coincide with some of the t_k 's. Compared with standard Euler time stepping methods, this is an essential advantage of this numerical technique.

Now, with exactly the same technique used for problem (P), we can prove that J_σ has partial derivatives and that

$$\frac{\partial J_\sigma}{\partial s_i}(u) = -\kappa_i \left[\int_0^{s_i} \int_\Omega \partial_t y_0(x, t - s_i) \varphi_\sigma(x, t) dx dt + \int_{s_i}^T \int_\Omega \partial_t y_\sigma(x, t - s_i) \varphi_\sigma(x, t) dx dt \right] \quad (20)$$

$$\frac{\partial J_\sigma}{\partial \kappa_i}(u) = \nu \kappa_i + \int_0^{s_i} \int_\Omega y_0(x, t - s_i) \varphi_\sigma(x, t) dx dt + \int_{s_i}^T \int_\Omega y_\sigma(x, t - s_i) \varphi_\sigma(x, t) dx dt. \quad (21)$$

The proof of existence of partial derivatives can be done following the same steps as for the continuous case. In a first step, we compute the partial derivatives of the discrete state as in Theorem 2.2. The key estimate (9) is replaced by the stability estimates in [16, Corollary 4.8]; the limit in (10) is also valid, since $\mathcal{Y}_\sigma^1 \hookrightarrow W^{1,q}(0, T; Y_h)$. Finally, we can pass to the limit in the linearized discrete equation taking into account that the discretization parameters (h, τ) are fixed, so we are working in a finite dimensional space. The expressions for the derivatives of the discrete functional follow from the chain rule as in the proof of Theorem 2.3.

Remark 2. In recent contributions to PDE control, discontinuous Galerkin (dG) methods became quite popular, [15]. We are able to discretize both the state equation and the adjoint state equation using the same set of discontinuous Galerkin elements dG(0), cf. [15, Eqs. (18) and (20)] and to derive expressions for the partial derivatives of the resulting discrete functional. However, the partial derivatives of the discrete objective functional are not everywhere continuous. The reason is the following:

To simplify the exposition, suppose that $\tau_k = \tau$ for all $k = 1, \dots, N_\tau$. Then, the control-to-discrete-state mapping is not differentiable at the nodes of the time mesh. Notice that the technique used in Theorem 2.2 cannot be applied because the discrete states are piecewise constant in time and $\mathcal{Y}_\sigma^0 \not\hookrightarrow W^{1,q}(0, T; Y_h)$, so the derivative with respect to time of the discrete state can not be identified with a function in $L^q(Q)$. Taking advantage of the fact that we are dealing with a finite dimensional problem, the partial derivatives of the discrete state with respect to the delays can be computed for any $t \neq t_k$, but jump discontinuities will appear at the nodes of the time mesh.

These jump discontinuities are inherited by the partial derivatives of the discrete functional. The expressions we obtain for the derivatives of the discrete functional are

formally the same as (20) and (21) if we identify the time derivatives of elements in \mathcal{Y}_σ^0 with combinations of Dirac measures centered at the time nodes. This leads to the discontinuities in the partial derivatives of J_σ with respect to the delays.

4. Examples

The aim of this section is to confirm that optimizing time delays in nonlinear parabolic delay equations is a useful concept. In particular, we demonstrate that oscillatory patterns can be achieved by an associated feedback control. In this way, our method is also some contribution to the topic of “learning controller”.

In our test examples, we do not restrict ourselves to problem (P). We will start with an example for a related ordinary differential delay equation. They are covered by our parabolic problem as particular case. It might be useful to first solve an ODE control problem and take the obtained result as initial guess for the solution of the associated PDE control problem. In addition, in the case of ordinary differential equations the graphs of the desired state and the computed optimal state can be graphically better compared.

Moreover, in the context of approximating periodic states of parabolic delay equations, we also consider a problem with slightly changed “shifted” objective functional as suggested in [10]; see examples 4.3 and 4.4 below.

To perform the optimization numerically, we use the MATLAB code `fmincon` with the option (`'SpecifyObjectiveGradient', true`) that needs the gradient of the function to be minimized. This code uses subroutines for calculating the functions $u \mapsto J_\sigma(u)$ and $u \mapsto \nabla J_\sigma(u)$. Both functions are evaluated by solving the discretized state equation and adjoint equation, respectively, according to the methods explained in the last section.

Since the code `fmincon` will in general find a local minimum, we performed several solves with different initial points to have a better chance for finding a global minimum.

In all our examples we focus on the non-monotone non-linearity

$$R(y) = y(y - 0.25)(y - 1)$$

and fix $T = 80$. We take $\nu = 0$, and impose the bounds $0 \leq s_i \leq T$, $|\kappa_i| \leq 1000$ for $i = 1 : m$. Figures 1 and 2 show the states up to $t = 2T$ to confirm that the obtained solutions exhibit a stable behavior for $t > T$.

Example 4.1. We start with one example for an ordinary differential delay equation (ODE). This fits in our setting as long as y_0 and R are constant with respect to x , because then the equation (5) reduces to an the ODE. We consider the ODE with delay

$$y'(t) + R(y) = \sum_{i=1}^m \kappa_i y(t - s_i) \text{ for } t \in (0, T], \quad y(t) = y_0(t), \text{ if } t \leq 0 \quad (22)$$

for $y : [-b, T] \rightarrow \mathbb{R}$, where $y_0 : [-b, 0] \rightarrow \mathbb{R}$ is given and $R : \mathbb{R} \rightarrow \mathbb{R}$ is the given reaction term.

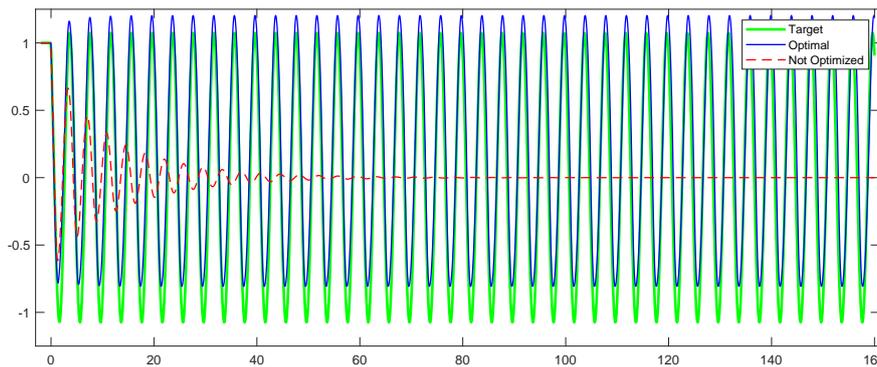


Figure 1. Example 4.1; Target state (green), optimal state (blue), and uncontrolled state (red).

We select the target state y_Q solving the linear delay equation

$$y'(t) = -\frac{\pi}{2}y(t-1) \text{ in } [0, T], \quad y(t) = 1 \text{ in } [-1, 0].$$

This function exhibits a stable oscillatory behavior; displayed as green curve in Fig. 1. A nice discussion of this particular equation can be found in Erneux [17].

For $m = 1$ and an appropriate choice of the parameters $u = (s, \kappa)$, we want to mimic that behavior by the solution of the *nonlinear* delay equation (22) with initial data $y_0(t) = 1$.

For the choice $s = 1$ and $\kappa = -\pi/2$, the state exhibits an oscillatory behavior, but $|y_u|$ decays in time, see the red dashed curve in Fig. 1. Our optimization problem is to minimize

$$J(s, \kappa) = \frac{1}{2} \int_0^T (y_u(t) - y_Q(t))^2 dt \quad (23)$$

subject to the state equation (22) and $0 \leq s \leq T$ and $|\kappa| \leq 1000$. Numerically, we obtained the solution $\bar{u} = (\bar{s}, \bar{\kappa})$ with

$$\bar{s} = 1.2409, \quad \bar{\kappa} = -1.7668$$

and an associated value $J(\bar{u}) = 1.8701$ of the objective functional. The gradient of J at the computed solution has the norm $|\nabla J(\bar{u})| = 3.8 \times 10^{-7}$. Figure 1 displays the optimal and the desired state in blue and green respectively. For comparison, $y_u(t)$ for $u = (1, -\pi/2)$ is plotted in dashed red. We had to use 2^{12} time steps in the discretization to capture correctly the behaviour of the linear delay equation that defines the target state.

For all the next examples, we consider the data of Example 3 in [10]: We fix $\Omega = (-20, 20) \subset \mathbb{R}$. The initial function y_0 models an incoming traveling wave, namely

$$y_0(x, t) = \frac{1}{2} \left[1 - \tanh \left(\frac{x - vt}{2} \right) \right],$$

with $v = 0.25\sqrt{2}$. This kind of problems appear in chemical wave propagation; see [18]. We aim at steering the system to the target state shown in Fig. 2a

$$y_Q(x, t) = 3 \sin \left(t - \cos \left(\frac{\pi}{20}(x + 20) \right) \right).$$

For the discretization, we take 2^7 finite elements in space and 2^7 steps in time.

Example 4.2. We fix $m = 6$ and obtain the optimal parameters shown in Table 1. A graph of the optimal state is shown in Fig. 2b.

i	\bar{s}_i	$\bar{\kappa}_i$
1	0.0000	0.9846
2	0.9367	-1.5039
3	6.7481	0.4542
4	28.3843	-2.2799
5	32.2258	3.7013
6	39.8133	-1.3844

Table 1. Example 4.2: Computed optimal result.

For these values, we have computed an optimal value $J(\bar{u}) = 4209.3$. This value is quite large, but note that the measure of $Q = (-20, 20) \times (0, 80)$ is equal to 3200. Therefore, the function $y \equiv 1$ has a norm square of 3200 in $L^2(Q)$.

Notice that the lower constraint for the delays is achieved, since $\bar{s}_1 = 0$, and $\sum_{i \neq 1} \kappa_i = -1.0127$, which is quite close to $-\kappa_1$. This somehow resembles the original Pyragas feedback form, since the term $y(x, t) = y(x, t - s_1)$ appears in the right-hand side of the partial differential equation, cf. also the subsection on Pyragas type control below. First order optimality conditions are satisfied: we obtain that $\partial_{s_1} J(\bar{u}) = 486 \geq 0$, remember \bar{s}_1 attains the lower constraint, and the maximum of the absolute value of the rest of the components of the gradient is 2.0×10^{-4} .

Objective functional with shift in the target If a given periodicity of the state is desired, then two states with the same period should be considered as equal if they differ only by a time shift. For instance, the functions $t \mapsto \sin(t)$ and $t \mapsto \sin(t + \pi)$ should be considered as equal. This is natural, since the time until developing an oscillatory behavior may depend on the selected delays. This inherent shift in time is unavoidable and makes the minimization of standard quadratic tracking type functionals difficult.

Therefore, in [10] it was suggested to include a shift ς in the target state y_Q . Then the target can be adjusted to the computed states during the numerical algorithm. In view of this, we will minimize now the shifted functional

$$J(u, \varsigma) = \frac{1}{2} \int_0^T (y_u(x, t) - y_Q(x, t - \varsigma))^2 dx dt \quad (24)$$

simultaneously with respect to $u \in U_{ad}$ and $\varsigma \in \mathbb{R}$.

We assume that the desired state y_Q is time-periodic with period $p > 0$. Then we might impose the additional constraint $\varsigma \in [0, p]$ that shows the existence of an optimal

shift by compactness. However, by periodicity, this constraint can be skipped and is numerically not needed.

The associated optimality conditions are obtained by minor modification. It is easy to see that, for given (u, ς) , the adjoint state φ is the solution of the equation

$$\begin{cases} -\partial_t \varphi - \Delta \varphi + R'(y_u) \varphi &= y(x, t) - y_Q(x, t - \varsigma) + \sum_{i=1}^m \kappa_i \varphi(x, t + s_i) & \text{in } Q \\ \partial_n \varphi(x, t) &= 0 & \text{on } \Sigma \\ \varphi(x, t) &= 0 & \text{if } t \geq T. \end{cases}$$

The expressions for the derivatives with respect to the delays and the weights are the same as the ones given in Theorem 2.3. The partial derivative with respect to the shift ς is

$$\frac{\partial J}{\partial \varsigma}(u, \varsigma) = \int_0^T \int_{\Omega} (y_u(x, t) - y_Q(x, t - \varsigma)) \frac{\partial y_Q}{\partial t}(x, t - \varsigma) dx dt. \quad (25)$$

Example 4.3. We take the same data as in Example 4.2, fix $m = 2$ delays, and minimize the shifted objective functional (24). Note that the desired function y_Q has the time period 2π .

The result is displayed in Table 2, the computed optimal state is shown in Fig. 2c. It is amazing, how good the desired pattern is approximated with only two time delays.

i	\bar{s}_i	$\bar{\kappa}_i$
1	2.2785	-8.2564
2	4.8126	-5.2898
Target shift $\bar{\varsigma} = 2.3775$		

Table 2. Example 4.3 (shifted functional): Optimal result

In this case, `fmincon` computed as optimal value $J(\bar{u}, \bar{\varsigma}) = 2114.5$ with gradient $|\nabla J(\bar{u}, \bar{\varsigma})| = 1.1 \times 10^{-6}$; It is remarkable that the shift essentially improved the numerical result of Example 4.2. Moreover, the computed periodic pattern remains stable after $t = 80$.

In [10] it is also suggested to change the objective functional to

$$\partial J(u, \varsigma) = \int_{T/2}^T \int_{\Omega} (y_u(x, t) - y_Q(x, t - \varsigma))^2 dx dt$$

because it is reasonable to assume that it takes some time to transfer the incoming traveling wave y_0 into a periodic solution. Using this new functional and increasing the number of time delays to $m = 8$, the objective value can be reduced down to $J(\bar{u}, \bar{\varsigma}) = 218.75$.

Pyragas type feedback control Finally, we investigate the approximation of oscillatory patterns that are characteristic for Pyragas type feedback control as in (1),

$$\begin{cases} \partial_t y - \Delta y + R(x, t, y) = \sum_{i=1}^m \kappa_i (y(x, t - s_i) - y(x, t)) & \text{in } Q \\ \partial_n y = 0 & \text{on } \Sigma \\ y(x, t) = y_0(x, t) & \text{in } Q^-. \end{cases} \quad (26)$$

We want to design a feedback controller by adjusting finitely many time delays and associated weights minimizing the shifted functional (24).

The adjoint state equation in this case is

$$\begin{cases} -\partial_t \varphi - \Delta \varphi + R'(y_u) \varphi = y(x, t) - y_Q(x, t - \varsigma) \\ \quad + \sum_{i=1}^m \kappa_i (\varphi(x, t + s_i) - \varphi(x, t)) & \text{in } Q \\ \partial_n \varphi(x, t) = 0 & \text{on } \Sigma \\ \varphi(x, t) = 0 & \text{if } t \geq T. \end{cases}$$

The expressions for the derivatives with respect to the delays and the shift are the same as the ones given in equations (11) and (25), while the derivative with respect to the weight is given by the expression

$$\frac{\partial J}{\partial \kappa_i}(u) = \nu \kappa_i + \int_Q \varphi_u(x, t) (y_u(x, t - s_i) - y_u(x, t)) dx dt.$$

Example 4.4. With the same data as in examples (4.2), we fix $m = 4$ and obtain the optimal parameters shown in Table 3. A plot of the optimal state is displayed in Fig. 2d. For these values, we computed an optimal value $J(\bar{u}, \bar{\varsigma}) = 3763.4$ with $|\nabla J(\bar{u}, \bar{\varsigma})| = 4.8 \times 10^{-4}$.

i	\bar{s}_i	$\bar{\kappa}_i$
1	1.8308	-2.1661
2	7.0918	2.2636
3	28.3354	-1.7753
4	36.1215	1.7550
Target shift $\bar{\varsigma} = -2.5013$		

Table 3. Example 4.4: Computed optimal result.

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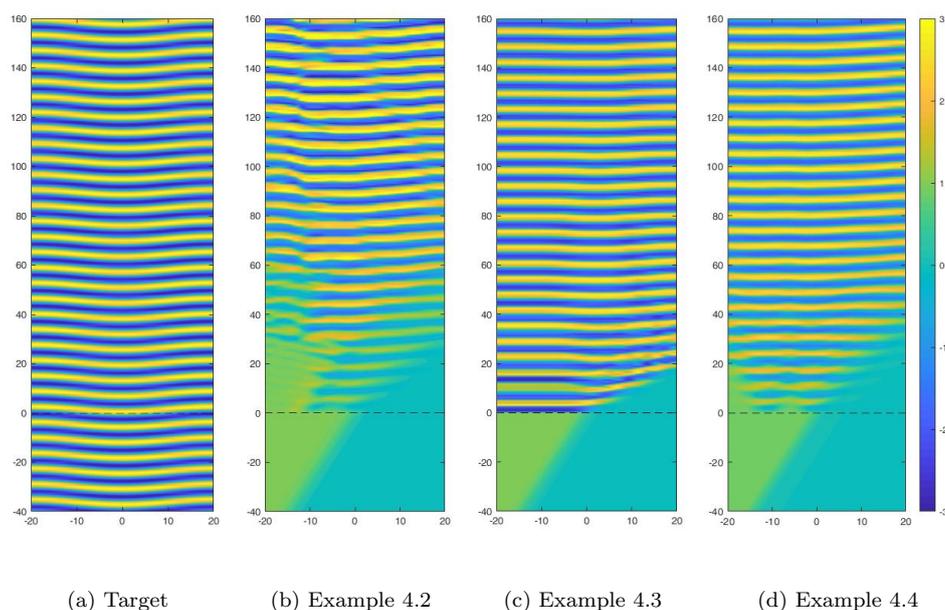


Figure 2. Examples 4.2-4.4: Target and optimal states. All functions are shown in $\Omega \times [-T/2, 2T]$.

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