

Some aspects of reachability for parabolic boundary control problems with control constraints

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Abstract A class of one-dimensional parabolic optimal boundary control problems is considered. The discussion includes Neumann, Robin, and Dirichlet boundary conditions. The reachability of a given target state in final time is discussed under box constraints on the control. As a mathematical tool, related exponential moment problems are investigated. Moreover, based on a detailed study of the adjoint state, a technique is presented to find the location and the number of the switching points of optimal bang-bang controls. Numerical examples illustrate this procedure.

Keywords Linear parabolic equation · Optimal boundary control problem · Box constraints · Reachability · Exponential moment problem

1 Introduction

In this paper, we consider aspects of controllability for optimal parabolic boundary control problems of the type

$$\min J(y, u) := \frac{1}{2} \int_0^1 (y(x, T) - y_d(x))^2 dx \quad (1.1)$$

subject to the one-dimensional heat equation

$$\begin{aligned} y_t(x, t) &= y_{xx}(x, t), & (x, t) &\in (0, 1) \times (0, T], \\ y_x(0, t) &= 0, & t &\in (0, T], \\ (By)(t) &= \beta u(t), & t &\in (0, T], \\ y(x, 0) &= 0, & x &\in (0, 1), \end{aligned} \quad (1.2)$$

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and to the pointwise control constraints

$$|u(t)| \leq 1 \quad \text{for almost all } t \text{ in } [0, T]. \quad (1.3)$$

In this setting, $T > 0$ and $\beta > 0$ are fixed constants, B denotes a certain differential operator specified below, and y_d is a fixed function of $L^2(0, 1)$. The function $u \in L^\infty(0, T)$ is the unknown boundary control.

We shall be concerned with the following three types of boundary conditions:

$$(By)(t) = y_x(1, t), \quad \beta = 1 \quad (\text{Neumann}), \quad (1.4)$$

$$(By)(t) = y_x(1, t) + \alpha y(1, t), \quad 0 < \alpha = \beta \quad (\text{Robin}), \quad (1.5)$$

$$(By)(t) = y(1, t), \quad \beta = 1 \quad (\text{Dirichlet}), \quad (1.6)$$

and we will denote the optimal control problems associated with the particular choice (1.4), (1.5) and (1.6) by (\mathcal{P}_N) , (\mathcal{P}_α) and (\mathcal{P}_D) , respectively.

Our interest to reconsider this very standard optimal control problem arose from numerical computations for Dirichlet boundary conditions, which were approximated by Robin boundary controls. This approximation process generated quite unexpected results. To interpret them, we had to answer the question whether the target function y_d was reached or not. From an analytical point of view, the answer is clear: y_d is reached, if $\|y(\cdot, T) - y_d\|_{L^2(0,1)} = 0$. Numerically, however, always $\|y(\cdot, T) - y_d\|_{L^2(0,1)} > 0$ is obtained, no matter if y_d is reachable or not.

In the case of Robin or Neumann control, it is well known that the optimal control is of bang-bang type if the optimal value of the functional J is positive, i.e. if the optimal state $y(\cdot, T)$ does not reach y_d . If the optimal control is not bang-bang, then y_d is attainable by controls satisfying the restrictions (1.3). This is the case of (restricted) reachability.

There is an extensive list of publications devoted to controllability of parabolic equations. We briefly sketch this issue in Sect. 4. However, we did not find results which could be applied to answer the question of restricted controllability for concrete examples.

In this paper, we discuss some ways to check numerically, if the target y_d is reachable or not. This is a delicate issue, and we are able to give only some partial answers. In Sect. 3 we verify by a numerical method, combined with precise estimations, that there is an optimal bang-bang control in a neighborhood of a computed bang-bang control and that the optimal value must be positive. In this way, we verify non-reachability. Moreover, we show for concrete examples that the optimal control has only one switching point. This was an open question since years, in particular, for a well-known benchmark example by Schittkowski [20], where the function $y_d(x) = (1 - x^2)/2$ is to be reached. We also address sufficient conditions for the existence of optimal bang-bang controls with finitely many switching points.

In Sect. 6, we present problems, where the numerical computations strongly indicate that y_d is attainable. We give an application of our results to the approximation of Dirichlet boundary controls. However, we were not able to prove that restricted reachability really takes place. Nevertheless, we discuss this example to show the specific difficulties of this problem.

2 Some known results on the control problem

Our experience with numerical computations revealed that the L^2 -norm of the optimal difference $y(\cdot, T) - y_d$ is very small. We usually obtained values smaller than $10^{-5} \dots 10^{-7}$. Therefore, finite difference or finite element methods cannot be used for the PDE to meet the necessary precision. This would require extremely fine meshes. Moreover, due to the accumulation of errors, we cannot trust in exact error estimates, even if the associated constants would be known.

Therefore, we applied the Fourier method to solving the heat equation, since we have reliable estimates for terminating these series.

The weak solution y of (1.2)—also denoted by $y(u)$ in order to stress that the *state* y belongs to *control* u —is given by the formula

$$y(x, t) = \beta \int_0^t G(x, 1, t - s)u(s) ds,$$

where G is the Green’s function associated with the parabolic boundary value problem. Expressed in this form, y is also called *generalized solution*. The Green’s function is given by the following infinite series:

$$G(x, \xi, t) = \begin{cases} 1 + \sum_{n=1}^\infty y_n(x)y_n(\xi)e^{-n^2\pi^2t} & \text{(Neumann b.c.)}, \\ \sum_{n=1}^\infty v_n(x)v_n(\xi)e^{-\mu_n^2t} & \text{(Robin b.c.)}, \\ \sum_{n=1}^\infty \varphi_n(x)(-\varphi'_n(\xi))e^{-v_n^2t} & \text{(Dirichlet b.c.)}, \end{cases} \tag{2.1}$$

where $\{\mu_n\}_{n \in \mathbb{N}}$ is the non-decreasing sequence of positive solutions of $\mu \tan(\mu) = \alpha$, $v_n = (n + 1/2)\pi$, and $v_n(x) := N_n^{-1/2} \cos(\mu_n x)$, $N_n := 1/2 + \sin(2\mu_n)/4\mu_n = \int_0^1 \cos^2(\mu_n x) dx$, $y_n(x) := \sqrt{2} \cos(n\pi x)$, $\varphi_n(x) = \sqrt{2} \cos(v_n x)$ are the complete orthonormal sequences of eigenfunctions of the 1-D Laplace operator corresponding to negative eigenvalues $\{-\lambda_n\}_{n \in \mathbb{N}}$, $\lambda_n = \{n^2\pi^2, \mu_n^2, v_n^2\}$:

$$-w_{xx} = \lambda_n w \quad \text{in } [0, 1], \quad w_x(0) = 0, \quad Bw = 0,$$

(see [11, 23], [21, Theorem 2.1]). Unlike the Neumann or Robin case, the symmetry $G(x, 1, t) = G(1, x, t)$, $x \in [0, 1], t \in [0, T]$, of the Green’s function is not true for the problem of Dirichlet boundary control. Let us introduce the linear continuous operator $S_T : L^2(0, T) \rightarrow L^2(0, 1)$,

$$(S_T u)(x) = \beta \int_0^T G(x, 1, T - s)u(s) ds \tag{2.2}$$

(see [9, 22]) and its adjoint operator $S_T^* : L^2(0, 1) \rightarrow L^2(0, T)$,

$$(S_T^* v)(t) = \beta \int_0^1 G(\xi, 1, T - t)v(\xi) d\xi. \tag{2.3}$$

Moreover, we define the set of feasible controls

$$U_{ad} := \{v \in L^2(0, T) \mid |v| \leq 1 \text{ a.e. in } [0, T]\}.$$

Then we have $y(x, T) = (S_T u)(x)$ and the optimal control problem can be written as follows: Find $\bar{u} \in U_{ad}$ such that

$$\|S_T \bar{u} - y_d\|_{L^2(0,1)}^2 = \min_{u \in U_{ad}} \|S_T u - y_d\|_{L^2(0,1)}^2. \quad (2.4)$$

Now, it follows by standard arguments that there exists an optimal control \bar{u} for (2.4), and hence for the problem (1.1)–(1.3). Moreover, we deduce that this control must satisfy the variational inequality

$$\langle S_T^*(S_T \bar{u} - y_d), u - \bar{u} \rangle_{L^2(0,T)} \geq 0 \quad \forall u \in U_{ad}, \quad (2.5)$$

where $\langle \cdot, \cdot \rangle$ is used to denote scalar products. By convexity, this variational inequality is also sufficient for optimality.

Remark 2.1 For convenience, from now on, we denote S_T and S_T^* by S and S^* respectively, if it is clear from the context, which final time T is meant.

The images $S_T^* v$ can be interpreted as generalized solutions to adjoint initial-boundary value problems. We do not make use of this fact in our analysis, since we only rely on the series representation (2.3) of $S_T^* v$. Nevertheless, we mention the associated adjoint equations for convenience:

In the Neumann or Robin case there holds $(S^* v)(t) = \beta p(1, t)$, where $p \in L^2([0, 1] \times [0, T])$ is the generalized solution of the adjoint equation

$$\begin{aligned} -p_t(x, t) &= p_{xx}(x, t), & (x, t) &\in (0, 1) \times (0, T], \\ p_x(0, t) &= 0, & (Bp)(t) &= 0, \quad t \in (0, T], \\ p(x, T) &= v(x), & x &\in [0, 1], \end{aligned}$$

cf. [22]. In the Dirichlet case, it holds $(S^* v)(t) = p_x(1, t)$, [13]. Inserting $v = S\bar{u} - y_d = \bar{y}(\cdot, T) - y_d$, we deduce from (2.5) the following optimality conditions:

Theorem 2.2 *A control $\bar{u} \in U_{ad}$ and its corresponding state \bar{y} are optimal for the boundary control problem (1.1)–(1.3), if and only if \bar{u} satisfies the variational inequality*

$$\langle \beta p(1, \cdot), u - \bar{u} \rangle_{L^2(0,T)} \geq 0, \quad \forall u \in U_{ad}, \quad (2.6)$$

for (\mathcal{P}_α) and (\mathcal{P}_N) , and

$$\langle p_x(1, \cdot), u - \bar{u} \rangle_{L^2(0,T)} \geq 0, \quad \forall u \in U_{ad}, \quad (2.7)$$

for (\mathcal{P}_D) , where p is the generalized solution of the adjoint state equation

$$\begin{aligned} -p_t(x, t) &= p_{xx}(x, t), & (x, t) &\in (0, 1) \times (0, T], \\ p_x(0, t) &= 0, & t &\in (0, T], \\ (Bp)(t) &= 0, & t &\in (0, T], \\ p(x, T) &= \bar{y}(x, T) - y_d(x), & x &\in [0, 1]. \end{aligned} \quad (2.8)$$

A standard pointwise discussion of the variational inequality (2.6) shows that

$$\bar{u}(t) = \begin{cases} -1 & \text{when } \beta p(1, t) > 0, \\ +1 & \text{when } \beta p(1, t) < 0 \end{cases} \tag{2.9}$$

must hold for almost all $t \in [0, T]$. Therefore, the behavior of \bar{u} depends on the number and location of the roots of $p(1, t)$ in $[0, T]$. Analogously, (2.7) implies a.e. on $[0, T]$

$$\bar{u}(t) = \begin{cases} -1 & \text{when } p_x(1, t) > 0, \\ +1 & \text{when } p_x(1, t) < 0, \end{cases} \tag{2.10}$$

so that the roots of $p_x(1, t)$ determine the form of \bar{u} . In general, the set of all associated roots might have positive measure and can be very irregular. However, for Neumann and Robin boundary control problems, the following well known theorem reveals the structure of this set:

Theorem 2.3 ([10]) (Countable bang-bang principle) *Let \bar{u} be optimal for the Neumann or Robin boundary control problem and let \bar{y} be the associated state. Suppose that $\|\bar{y}(\cdot, T) - y_d\|_{L^2(0, T)} > 0$. Then the function $p(1, \cdot)$ has at most countably many zeros $0 < t_1 < t_2 < \dots < t_i < \dots < T$ in $[0, T]$, which can accumulate only at $t = T$. If $\frac{dp}{dt}(1, t_i) \neq 0$ for all $i \in \mathbb{N}$, then, either $\bar{u}(t) = (-1)^i$ or $\bar{u}(t) = (-1)^{i+1}$ holds a.e. on $[t_i, t_{i+1}]$ for all relevant $i \in \mathbb{N}$.*

Definition 2.1 A value $\tau \in (0, T)$ is said to be a *switching point* of a bang-bang control u , if there exists $\varepsilon > 0$ such that $u(t) = -u(s) \forall t \in (\tau - \varepsilon, \tau), s \in (\tau, \tau + \varepsilon)$.

This theorem shows that optimal Neumann or Robin boundary controls must be of bang-bang type, unless the optimal value $J(\bar{y}, \bar{u})$ is zero. In other words, if the optimal control is not bang-bang, then the target state y_d is reachable by controls of U_{ad} . Therefore, if a numerically computed optimal control is not bang-bang, then this is some indication for exact restricted controllability. However, this is not a proof, since numerical effects might have perturbed the true optimal control. Notice that the functional J does not contain a Tikhonov type regularization term, hence numerical computations are not stable with respect to perturbations.

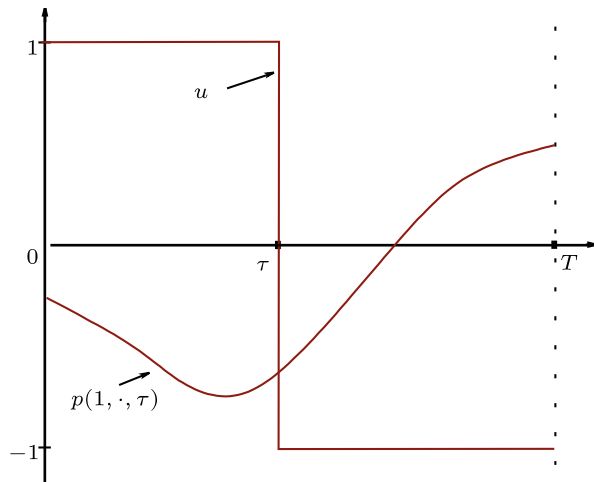
3 Verification of optimal bang-bang controls

3.1 The main theorem

In this section, we present a method, how the existence of optimal bang-bang controls and the non-reachability of y_d can be verified numerically. We begin with the Neumann boundary condition, since here the Green’s function is very easy to discuss.

In a first result, we show for a concrete problem that the optimal control is bang-bang with exactly one switching point. Later, in Sect. 5, we briefly discuss the case of more switching points.

Fig. 1 Assumed situation



For the numerical solution of the problem (1.1)–(1.3), the control was approximated by $n_t = 101$ step functions, using an equidistant partition of $[0, T]$ into $n_t - 1$ intervals. We truncated the infinite series (2.1) after an index N such that the remainder can be neglected for our purposes. In order to locate the switching point providing the minimal value of the functional J , we made use of the bisection method.

Let us first present our general idea for the following situation: For a given problem, thanks to numerical computations, we expect that the optimal control \bar{u} is bang-bang with only one switching point at an unknown value $\bar{\tau}$, $0 < \bar{\tau} < T$. Let us assume that \bar{u} is positive in $[0, \bar{\tau}]$. Then the optimal control should belong to the class of controls u that have the form

$$u(t) = u(t, \tau) := \begin{cases} 1 & \text{for } t < \tau, \\ -1 & \text{for } t > \tau. \end{cases} \tag{3.1}$$

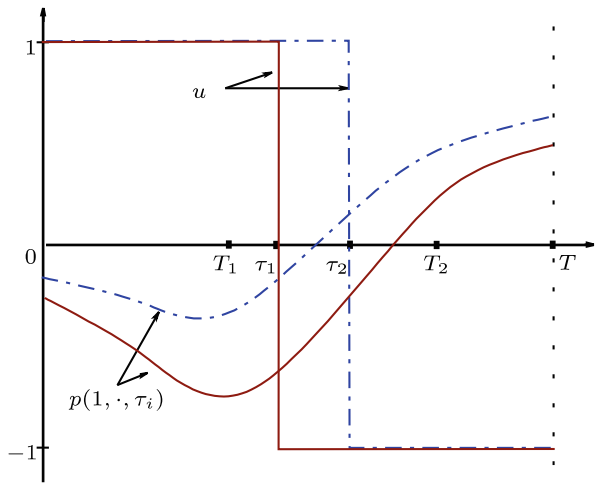
However, our assumption is based on numerical results, hence our expectation that \bar{u} has the form (3.1) is only a conjecture. Therefore, we try to verify that among those bang-bang controls there is really one that satisfies the optimality conditions.

Let $u = u(\cdot, \tau)$ be a result of the numerical optimization and denote the associated adjoint state by $p(x, \cdot, \tau)$. Our numerical experience with such problems shows that, even for very fine discretization, the switching point of the computed control does not exactly coincide with the root of $p(x, \cdot, \tau)$. Assume that we arrived at the situation presented in Fig. 1, which is now used to explain our main idea.

The computed adjoint state $p(1, \cdot, \tau)$ in Fig. 1 has exactly one zero at $t = t(\tau)$ located right of the switching point τ . In Fig. 2, we denote this computed switching point τ by τ_1 . Assume also that, by another computation, we have found a switching point $\tau_2 > \tau_1$ such that the adjoint state $p(1, \cdot, \tau_2)$ has a single root $t(\tau_2)$ located left of τ_2 .

We are going to show that $t(\tau)$ is a strongly monotone decreasing and continuous function of τ on $[\tau_1, \tau_2]$. Increasing the switching point τ will decrease the root $t(\tau)$ of p . We have $t(\tau_1) - \tau_1 > 0$ and $t(\tau_2) - \tau_2 < 0$ so that the intermediate value

Fig. 2 Illustration of the main idea



theorem ensures the existence of a value $\bar{\tau} \in [\tau_1, \tau_2]$, where $\bar{\tau} = t(\bar{\tau})$. The root of $p(1, \cdot, \bar{\tau})$ coincides with the switching point $\bar{\tau}$. If we show in addition that $p(1, \cdot, \bar{\tau})$ does not have any other root in $(0, T)$ and is negative on $(0, \bar{\tau})$, then $u(\cdot, \bar{\tau})$ satisfies the optimality conditions and is optimal.

Theorem 3.1 Assume the existence of values $0 \leq T_1 \leq \tau_1 < \tau_2 \leq T_2 \leq T$ with the following properties: The function $p(1, \cdot, \cdot)$ is continuously differentiable on $D := (T_1, T_2) \times [\tau_1, \tau_2]$,

$$p(1, \tau_1, \tau_1) < 0, \quad p(1, T_2, \tau_1) > 0, \tag{3.2}$$

$$p(1, \tau_2, \tau_2) > 0, \quad p(1, T_1, \tau_2) < 0, \tag{3.3}$$

$$\frac{\partial}{\partial t} p(1, t, \tau) > 0 \quad \forall (t, \tau) \in D, \tag{3.4}$$

$$\frac{\partial}{\partial \tau} p(1, t, \tau) > 0 \quad \forall (t, \tau) \in D. \tag{3.5}$$

Then, for all $\tau \in (\tau_1, \tau_2)$, the function $t \mapsto p(1, t, \tau)$ has a single root $t(\tau)$ between $t(\tau_1)$ and $t(\tau_2)$. There exists a unique fixed point $\bar{\tau}$ of the mapping $\tau \mapsto t(\tau)$ in (τ_1, τ_2) .

Proof The existence of the zeros $t(\tau_1), t(\tau_2)$ follows from the intermediate value theorem. Moreover

$$\tau_1 < t(\tau_1), \quad t(\tau_2) < \tau_2.$$

Let $\tau \in I := (\tau_1, \tau_2)$ be given. We first show the existence of a root $t(\tau)$ of $t \mapsto p(1, t, \tau)$ between $t(\tau_1)$ and $t(\tau_2)$. Notice that we do not have an information on the order of $t(\tau_1)$ and $t(\tau_2)$. We know that

$$p(1, t(\tau_1), \tau_1) = p(1, t(\tau_2), \tau_2) = 0.$$

Because of $\tau_1 < \tau < \tau_2$, the condition (3.5) of strong monotonicity yields

$$p(1, t(\tau_1), \tau) > 0 \quad \text{and} \quad p(1, t(\tau_2), \tau) < 0.$$

Therefore, by the intermediate value theorem, the function $t \mapsto p(1, t, \tau)$ has a root $t(\tau)$ between $t(\tau_1)$ and $t(\tau_2)$, and hence in (T_1, T_2) . This holds for all $\tau \in I$. The uniqueness of the root $t(\tau)$ in (T_1, T_2) is a consequence of (3.4).

It remains to show that the mapping $\tau \mapsto t(\tau)$ has a fixed point in I . By definition, $t(\tau)$ satisfies

$$p(1, t(\tau), \tau) = 0 \quad \forall \tau \in I.$$

In view of assumption (3.4), we can apply the implicit function theorem to infer that t is a continuously differentiable function of τ . From

$$\frac{d}{d\tau} p(1, t(\tau), \tau) = \frac{\partial}{\partial t} p(1, t(\tau), \tau) \cdot t'(\tau) + \frac{\partial}{\partial \tau} p(1, t(\tau), \tau) = 0$$

and (3.4)–(3.5) we deduce

$$t'(\tau) = - \frac{\frac{\partial}{\partial \tau} p(1, t(\tau), \tau)}{\frac{\partial}{\partial t} p(1, t(\tau), \tau)} < 0.$$

Consider now the function $g : \tau \mapsto t(\tau) - \tau$, $g : [\tau_1, \tau_2] \rightarrow \mathbb{R}$. By the differentiability of $t(\cdot)$, g is differentiable. In view of our assumptions on τ_1, τ_2 , g has different signs in the points τ_1 and τ_2 . Therefore, the intermediate function theorem yields the existence of a root $\bar{\tau}$ of g between τ_1 and τ_2 . This is the desired fixed point. Moreover, it holds

$$g'(\tau) = t'(\tau) - 1 < 0$$

in I , hence the fixed point is unique. □

The above theorem is a tool to confirm the existence of optimal bang-bang controls. To use it, we have to verify the differentiability of $p(1, t, \tau)$ with respect to both variables. Moreover, we must confirm by careful estimations that the assumptions (3.2)–(3.5) of the theorem are satisfied. Last but not least, we must guarantee that $p(1, t, \tau)$ does not have other roots in $(0, T)$ than $t(\tau)$, for all $\tau \in [\tau_1, \tau_2]$.

We work out these details now for the case of Neumann boundary control.

3.2 Neumann boundary control

The concrete function y_d we consider was introduced by Schittkowski [20], it is

$$y_d(x) = \frac{1}{2}(1 - x^2). \tag{3.6}$$

This function was frequently used in the literature to set up test examples for the numerical solution of optimal boundary control problems with Neumann or Robin boundary conditions and different values of the final time T . The numerical methods

delivered optimal controls of the type (3.1). But to our best knowledge it was never confirmed that the exact optimal control has this form. It was even not clear, if the optimal control has only finitely many switching points.

Our next goal is to answer these open questions for the particular choice (3.6).

3.2.1 Fourier expansion for $p(1, t, \tau)$

We first mention the formula

$$\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos(n\pi x) = \frac{\pi^2}{4} \left(x^2 - \frac{1}{3} \right),$$

which is essential for two reasons: First, we use it later in the estimations. Second, this series is very slowly convergent so that the knowledge of its exact value avoids a numerical evaluation, which is not useful to reach the high precision we need. We obtain for $u = u(t, \tau)$

$$\begin{aligned} (Su)(x) &= \int_0^T \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \cos(n\pi x) e^{-n^2\pi^2(T-s)} \right] u(s) ds \\ &= 2\tau - T + 2 \sum_{n=1}^{\infty} (-1)^n \cos(n\pi x) \left[\int_0^\tau e^{-n^2\pi^2(T-s)} ds - \int_\tau^T e^{-n^2\pi^2(T-s)} ds \right] \\ &= 2\tau - T + 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2\pi^2} \cos(n\pi x) [2e^{-n^2\pi^2(T-\tau)} - e^{-n^2\pi^2T} - 1] \\ &= 2\tau - T - \frac{1}{2} \left(x^2 - \frac{1}{3} \right) + 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2\pi^2} \cos(n\pi x) [2e^{-n^2\pi^2(T-\tau)} - e^{-n^2\pi^2T}]. \end{aligned}$$

Notice that all infinite series in this representation are rapidly converging for $\tau < T$.

To compute $p(1, t) = p(1, t, \tau) = S^*(Su(\cdot, \tau) - y_d)(t)$, we have to apply S^* on Su and y_d :

$$\begin{aligned} S^*(Su)(t) &= \int_0^1 \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \cos(n\pi \xi) e^{-n^2\pi^2(T-t)} \right] (Su)(\xi) d\xi \\ &= \int_0^1 \left\{ 2\tau - T - \frac{1}{2} \left[\xi^2 - \frac{1}{3} \right] \right. \\ &\quad \left. + 2 \sum_{n=1}^{\infty} (-1)^n e^{-n^2\pi^2(T-t)} \int_0^1 \cos(n\pi \xi) (Su)(\xi) d\xi \right\} d\xi \\ &= 2\tau - T + \sum_{n=1}^{\infty} e^{-n^2\pi^2(T-t)} \left[(-1)^{n+1} \int_0^1 \cos(n\pi \xi) \xi^2 d\xi \right. \\ &\quad \left. + \frac{2}{n^2\pi^2} (2e^{-n^2\pi^2(T-\tau)} - e^{-n^2\pi^2T}) \right], \end{aligned}$$

where we used the orthogonality of the system $\{\cos(n\pi \cdot)\}_{n \in \mathbb{N}}$ and $\int_0^1 \cos(n\pi x) dx = 0$. Thus

$$S^*(Su)(t) = 2\tau - T + 2 \sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} e^{-n^2\pi^2(T-t)} [2e^{-n^2\pi^2(T-\tau)} - e^{-n^2\pi^2T} - 1]. \tag{3.7}$$

Along with (3.7) and

$$\begin{aligned} S^*y_d(t) &= \frac{1}{2} \int_0^1 \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \cos(n\pi x) e^{-n^2\pi^2(T-t)} \right] (1 - \xi^2) d\xi \\ &= \frac{1}{2} \int_0^1 (1 - \xi^2) d\xi + \sum_{n=1}^{\infty} (-1)^n e^{-n^2\pi^2(T-t)} \int_0^1 \cos(n\pi \xi) (1 - \xi^2) d\xi \\ &= \frac{1}{3} - 2 \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2(T-t)}}{n^2\pi^2}, \end{aligned}$$

we finally obtain

$$p(1, t, \tau) = 2\tau - T - \frac{1}{3} + 2 \underbrace{\sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} e^{-n^2\pi^2(T-t)} [2e^{-n^2\pi^2(T-\tau)} - e^{-n^2\pi^2T}]}_{=: B_n(t, \tau)}. \tag{3.8}$$

It is easy to confirm that $p(1, \cdot, \cdot)$ is continuous in the set $\{(t, \tau) \mid 0 \leq t \leq T, 0 \leq \tau \leq T\}$ and continuously differentiable in its interior.

Moreover, $\frac{\partial p}{\partial \tau}$ and $\frac{\partial p}{\partial t}$ are positive in this set, hence $p(1, t, \tau)$ is strictly monotone increasing with respect to t and τ . This is a very strong property that only holds for the Neumann boundary condition, cf. also the illustration in Fig. 3. The discussion in the Robin case is more delicate, since the monotonicity of p will only hold in a neighborhood of the switching point.

Summarizing up, in the Neumann case the assumptions (3.4)–(3.5) of Theorem 3.1 are met for the function y_d defined in (3.6). It remains to verify the other assumptions of this theorem in concrete examples. We demonstrate this next.

3.2.2 Application of Theorem 3.1 to Neumann boundary control

We consider the following concrete setting:

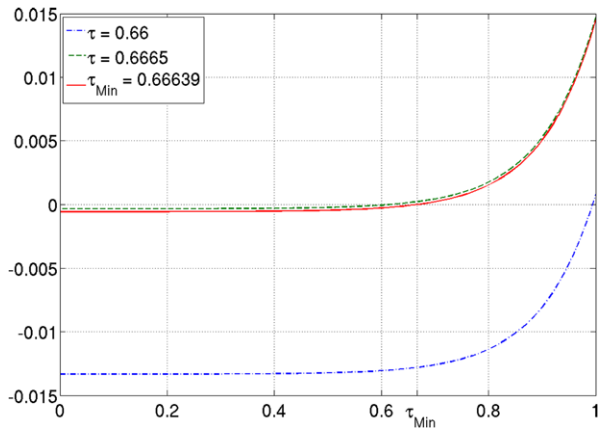
Example 1 We consider (\mathcal{P}_N) with y_d given by (3.6) and $T = 1$.

Let us apply Theorem 3.1 to this example. To verify its assumptions, we take

$$\tau_1 = 0.66, \quad \tau_2 = 0.6665, \quad T_1 = 0 \quad \text{and} \quad T_2 = T.$$

The situation is illustrated in Fig. 3. Our numerical computations delivered the switching point 0.66639. This point was computed for a discretization of the optimal control problem with $n_t = 101$.

Fig. 3 $p(1, \cdot, \tau)$ computed for $N = 5$, $\tau = 0.66, 0.6665$ and $\tau = \tau_{Min} = \bar{\tau}$



In the estimations below, we use the terms B_n introduced in (3.8).

Verification of (3.2) It is easy to confirm that $B_n > 0 \forall n \geq 1$. For $t = T_2 = T$ we obtain from (3.8), along with $2\tau_1 - T - \frac{1}{3} = 1.32 - 1 - \frac{1}{3} = -\frac{4}{300}$, that

$$\begin{aligned}
 p(1, T, \tau_1) &\geq 2\tau_1 - T - \frac{1}{3} + 2B_1(T, \tau_1) = -\frac{4}{300} + \frac{2}{\pi^2} [2e^{-\pi^2(1-0.66)} - e^{-\pi^2}] \\
 &> -\frac{4}{300} + \frac{2}{\pi^2} \cdot 0.0697 > 0.
 \end{aligned}$$

Conversely, for $t = \tau_1$ there holds

$$\begin{aligned}
 2 \sum_{n=1}^{\infty} B_n(\tau_1, \tau_1) &= 2 \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2(T-\tau_1)}}{n^2\pi^2} [2e^{-n^2\pi^2(T-\tau_1)} - e^{-n^2\pi^2T}] \\
 &< 2 \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2(T-\tau_1)}}{n^2\pi^2} 2e^{-n^2\pi^2(T-\tau_1)} \\
 &\leq 4e^{-2\pi^2(T-\tau_1)} \sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} = \frac{2}{3}e^{-2\pi^2(1-0.66)} < \frac{4}{300},
 \end{aligned}$$

hence $p(1, \tau_1, \tau_1) < 0$. Since $p(1, \cdot, \tau_1)$ is continuous on (τ_1, T) , there exists $t(\tau_1) \in (\tau_1, T)$ with $p(1, t(\tau_1), \tau_1) = 0$.

Verification of (3.3) In the same manner, we have $p(1, 0, \tau_2) < 0, p(1, \tau_2, \tau_2) > 0$.

Using $2\tau_2 - T - \frac{1}{3} = 1.333 - 1 - \frac{1}{3} = -\frac{1}{3000}$, we get for $t = T_1 = 0$,

$$\begin{aligned}
 2 \sum_{n=1}^{\infty} B_n(0, \tau_2) &= 2 \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2}}{n^2\pi^2} [2e^{-n^2\pi^2(1-0.6665)} - e^{-n^2\pi^2}] \\
 &\leq 4 \sum_{n=1}^{\infty} \frac{e^{-n^2\pi^2}}{n^2\pi^2} e^{-n^2\pi^2(1-0.6665)} \\
 &\leq 4 \sum_{n=1}^{\infty} \frac{e^{-\pi^2}}{n^2\pi^2} e^{-\pi^2(1-0.6665)} = \frac{2}{3}e^{-\pi^2(2-0.6665)} < \frac{1}{3000},
 \end{aligned}$$

and for $t = \tau_2 = 0.6665$,

$$\begin{aligned} p(1, \tau_2, \tau_2) &\geq 2\tau_2 - T - \frac{1}{3} + 2B_1(\tau_2, \tau_2) \\ &= -\frac{1}{3000} + \frac{2e^{-\pi^2(1-0.6665)}}{\pi^2} [2e^{-\pi^2(1-0.6665)} - e^{-\pi^2}] \\ &> -\frac{1}{3000} + 5.6 \cdot 10^{-4} > 0. \end{aligned}$$

Once again, from the continuity of $p(1, \cdot, \tau_2)$ on $(0, \tau_2)$ we deduce the existence of $t(\tau_2) \in (0, \tau_2)$, with $p(1, t(\tau_2), \tau_2) = 0$.

The inequalities (3.4) and (3.5) follow easily from the strong monotonicity of $p(1, \cdot, \tau)$ and $p(1, t, \cdot)$ for every $\tau \in [\tau_1, \tau_2]$ and $t \in (0, T)$. Hence $t(\tau_1)$, $t(\tau_2)$ are unique.

From Theorem 3.1, we obtain a unique value $\bar{\tau} \in (\tau_1, \tau_2)$ with $p(1, \bar{\tau}, \bar{\tau}) = 0$. For $\bar{\tau}$, the switching point of $u(\cdot, \bar{\tau})$ and the root of $p(1, t, \bar{\tau})$ coincide. Moreover, since $t \mapsto p(1, t, \bar{\tau})$ is strongly monotone on $(0, T)$, the root of $p(1, \cdot, \bar{\tau})$ is unique. Consequently, there is no need to check that $p(1, \cdot, \bar{\tau})$ does not have roots different from $\bar{\tau}$.

Thanks to these facts, we may now state the following result:

Theorem 3.2 *With $T = 1$ and $y_d(x) = \frac{1}{2}(1 - x^2)$, the Neumann boundary control problem (\mathcal{P}_N) admits an optimal bang-bang control \bar{u} of the form (3.1) with one single switching point $\bar{\tau}$ in $[0.66, 0.6665]$.*

Numerically we found $\bar{\tau}$ at 0.66639.

Remark 3.3 Though we found an optimal bang-bang control \bar{u} for the problem (\mathcal{P}_N) , it is still possible that $J(\bar{u}) = 0$, i.e. the case of exact restricted reachability might happen. However, from Theorem 4.5 it follows that y_d given by (3.6) is not attainable by controls satisfying (1.3). Therefore, $J(\bar{u}) > 0$ and \bar{u} is unique, since there cannot exist two different optimal bang-bang controls.

3.3 Robin boundary control

For a Robin boundary condition, the situation is more delicate. Let us investigate a similar setting as in the Neumann case. We use again the target function y_d defined in (3.6), the same set U_{ad} but a different final time.

3.3.1 Fourier expansion for $p(1, t, \tau)$

We have to consider now the second formula in the expression (2.1) of the Green's function. It is known that (see, for instance, Krabs [11])

$$0 < \mu_n < \pi \left(n - \frac{1}{2} \right), \quad n\pi < \mu_{n+1}, \quad (3.9)$$

and

$$\lim_{n \rightarrow \infty} [\mu_n - (n - 1)\pi] = 0.$$

Following the treatment of the Neumann boundary control problem, let $u = u(t, \tau)$ be a bang-bang control of the form (3.1). Then

$$\begin{aligned} (Su)(x) &= \alpha \sum_{n=1}^{\infty} v_n(1)v_n(x) \left[\int_0^{\tau} e^{-\mu_n^2(T-s)} ds - \int_{\tau}^T e^{-\mu_n^2(T-s)} ds \right] \\ &= \alpha \sum_{n=1}^{\infty} \frac{1}{\mu_n^2} v_n(1)v_n(x) [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2T} - 1] \\ &= \alpha \sum_{n=1}^{\infty} \frac{1}{\mu_n^2} v_n(1)v_n(x) [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2T}] - 1, \end{aligned} \tag{3.10}$$

where we used the explicit representation

$$\alpha \sum_{n=1}^{\infty} \mu_n^{-2} v_n(1)v_n(x) \equiv 1.$$

Next, we derive the expression for $p(1, t, \tau) = S^*(Su(\cdot, \tau) - y_d)(t)$. Applying S^* to Su , we obtain from (3.10)

$$\begin{aligned} S^*(Su)(t) &= \alpha \int_0^1 G(1, \xi, T - t)(Su)(\xi) d\xi \\ &= \alpha \sum_{n=1}^{\infty} v_n(1)e^{-\mu_n^2(T-t)} \int_0^1 v_n(\xi) \\ &\quad \times \left[\alpha \sum_{m=1}^{\infty} \frac{1}{\mu_m^2} v_m(1)v_m(\xi) [2e^{-\mu_m^2(T-\tau)} - e^{-\mu_m^2T}] - 1 \right] d\xi. \end{aligned}$$

The orthogonality of the system $\{v_n(\cdot)\}_n$ yields

$$\begin{aligned} S^*(Su)(t) &= \alpha^2 \sum_{n=1}^{\infty} \frac{1}{\mu_n^2} v_n^2(1)e^{-\mu_n^2(T-t)} [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2T}] \\ &\quad - \alpha \sum_{n=1}^{\infty} v_n(1)e^{-\mu_n^2(T-t)} \int_0^1 v_n(\xi) d\xi \\ &= \alpha^2 \sum_{n=1}^{\infty} \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) e^{-\mu_n^2(T-t)} [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2T} - 1], \end{aligned} \tag{3.11}$$

according to the definition of v_n and by $\mu_n \sin(\mu_n) = \alpha \cos(\mu_n)$. By the identity

$$\int_0^1 \cos(\mu_n \xi)(1 - \xi^2) d\xi = 2 \frac{\sin(\mu_n) - \mu_n \cos(\mu_n)}{\mu_n^3}, \tag{3.12}$$

we get for $y_d(x) = (1 - x^2)/2$

$$\begin{aligned} (S^* y_d)(t) &= \alpha \sum_{n=1}^{\infty} \frac{1}{N_n \mu_n^3} \cos(\mu_n) e^{-\mu_n^2(T-t)} [\sin(\mu_n) - \mu_n \cos(\mu_n)] \\ &= \sum_{n=1}^{\infty} \frac{1}{N_n} \cos^2(\mu_n) e^{-\mu_n^2(T-t)} \left[\frac{\alpha^2}{\mu_n^4} - \frac{\alpha}{\mu_n^2} \right], \end{aligned} \tag{3.13}$$

where again $\mu_n \sin(\mu_n) = \alpha \cos(\mu_n)$ was used. Finally, it follows from (3.11) and (3.13) that

$$\begin{aligned} p(1, t, \tau) &= \alpha^2 \sum_{n=1}^{\infty} \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) e^{-\mu_n^2(T-t)} [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2 T} - 1] \\ &\quad - \sum_{n=1}^{\infty} \frac{1}{N_n} \cos^2(\mu_n) e^{-\mu_n^2(T-t)} \left[\frac{\alpha^2}{\mu_n^4} - \frac{\alpha}{\mu_n^2} \right] \\ &= \alpha^2 \sum_{n=1}^{\infty} \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) e^{-\mu_n^2(T-t)} [2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2 T} - \mu_n^{-2} - 1 + \alpha^{-1}]. \end{aligned} \tag{3.14}$$

Since the series in (3.14) converges rapidly, only the first few terms have to be evaluated numerically.

3.3.2 Application of Theorem 3.1 to the example by Schittkowski

Example 2 As in Schittkowski [20], we choose in (\mathcal{P}_α) the function y_d as in (3.6), $T = 1.58$ and $\alpha = 1$.

The numerical result of the optimization method is very close to a bang-bang control with switching point at 1.3293 and optimal objective value of the order 10^{-5} , cf. Fig. 10. To verify that the exact optimal control is of the type (3.1), we apply our method with

$$\tau_1 = 1.329, \quad \tau_2 = 1.3294, \quad T_1 = 1.2 \quad \text{and} \quad T_2 = 1.42.$$

We shall discuss this choice below and verify the assumptions of Theorem 3.1. Two main difficulties occur, cf. also Fig. 4. Here, $p(1, t)$ is not monotone. Moreover, we have to verify the $p(1, t)$ remains positive after T_2 , in particular at $t = T$.

Fig. 4 $p(1, \cdot, \tau)$ computed for $\alpha = 1, N = 5, \tau = 1.329, 1.3294$ and $\tau = \tau_{Min} = \bar{\tau}$

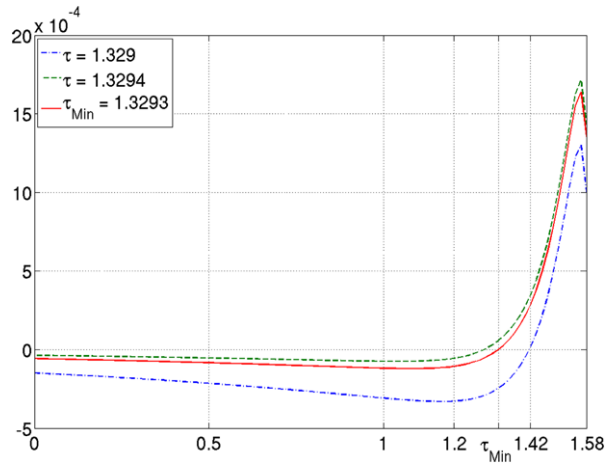


Table 1 μ_n for $n = 1, \dots, 5$

n	1	2	3	4	5
μ_n	0.86033359	3.42561846	6.43729818	9.5293344	12.6452872

For $\alpha = 1$, (3.14) reduces to

$$p(1, t, \tau) = \sum_{n=1}^{\infty} \underbrace{N_n^{-1} \mu_n^{-2} \cos^2(\mu_n) e^{-\mu_n^2(T-t)}}_{C_n(t)} \left[\underbrace{2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2 T} - \mu_n^{-2}}_{D_n(\tau)} \right].$$

Notice that $C_n(t)$ is always nonnegative, while, for $\tau < T$, $D_n(\tau)$ is nonnegative for the first few n and negative for all other n , as we shall see below. Moreover, the D_n do not depend on t . All this will be heavily used in the sequel.

Some preparatory inequalities From

$$N_n = \frac{1}{2} + \frac{\sin(2\mu_n)}{4\mu_n} = \frac{1}{2} + \frac{2 \sin(\mu_n) \cos(\mu_n)}{4\mu_n} = \frac{1}{2} + \frac{2 \sin^2(\mu_n)}{4} \geq \frac{1}{2} \tag{3.15}$$

and (3.9) we get for all $n \in \mathbb{N}$

$$C_n(t) = \frac{\cos^2(\mu_n)}{N_n \mu_n^2} e^{-\mu_n^2(T-t)} \leq \frac{2}{(n-1)^2 \pi^2} e^{-(n-1)^2 \pi^2 (T-t)}. \tag{3.16}$$

We have to evaluate the infinite series for $p(1, t, \tau)$ numerically. To gain precise information on its sign, we shall split this series into the sum of the first three items and the remainder. This remainder will be estimated, which is a little bit tedious but fairly easy. For the convenience of the reader who wants to check our estimates, the values of μ_n are given in Table 1, for $n = 1, \dots, 5$.

Next, we derive some useful estimates for $D_n(\tau)$ and $C_n(t)$ for $n \geq 4, t \in [T_1, T_2]$ and $\tau \in [\tau_1, \tau_2]$. As a conclusion of (3.16), we obtain

$$C_n(t) \leq \frac{2}{9\pi^2} (e^{-3\pi^2(T-t)})^{n-1} = \frac{2}{9\pi^2} q_t^{n-1} \quad \forall n \geq 4, \forall t \in [0, T),$$

where $q_t := e^{-3\pi^2(T-t)} < 1$. Further,

$$D_n(\tau) = 2e^{-\mu_n^2(T-\tau)} - e^{-\mu_n^2 T} - \mu_n^{-2} < 0 \quad \forall n \geq 4, \forall \tau \in [\tau_1, \tau_2]. \tag{3.17}$$

Certainly, it suffices to show $2e^{-\mu_n^2(T-\tau)} - \mu_n^{-2} < 0$. Applying the logarithm, this is equivalent to $2 \ln(\mu_n) < \mu_n^2(T - \tau) - \ln(2)$. The right-hand side satisfies, for $n \geq 4$,

$$\begin{aligned} \mu_n^2(T - \tau) - \ln(2) &\geq \mu_n(n - 1)\pi(1.58 - 1.3294) - \ln(2) \\ &\geq \mu_n \frac{3\pi}{4} - \ln(2) > 2\mu_n - \ln(2). \end{aligned}$$

The left-hand side can be estimated by

$$2 \ln(\mu_n) \leq 2(\mu_n - 1) = 2\mu_n - 2 < 2\mu_n - \ln(2).$$

This shows (3.17). Moreover

$$|D_n(\tau)| \leq e^{-\mu_n^2 T} + \frac{1}{\mu_n^2} \leq e^{-9\pi^2 \cdot 1.58} + \frac{1}{9\pi^2} < 1.13 \cdot 10^{-2} \quad \forall n \geq 4, \forall \tau \in [\tau_1, \tau_2]. \tag{3.18}$$

Now we are able to estimate the remainder: From (3.16) and (3.18) we obtain

$$\sum_{n=4}^{\infty} C_n(t) |D_n(\tau)| \leq \frac{2.26}{9\pi^2} \cdot 10^{-2} \cdot \sum_{n=3}^{\infty} q_t^n = c_0 \cdot \left[\frac{1}{1 - q_t} - 1 - q_t - q_t^2 \right], \tag{3.19}$$

where $c_0 := \frac{2.26}{9\pi^2} \cdot 10^{-2} < 2.545 \cdot 10^{-4}$. Evaluating this estimate at $t = T_1, \tau_1, \tau_2$ and T_2 , we get

$$\sum_{n=4}^{\infty} C_n(t) |D_n(\tau)| < \begin{cases} 5.345e - 19, & t = T_1, \\ 5.285e - 14, & t = \tau_1, \\ 5.477e - 14, & t = \tau_2, \\ 1.727e - 10, & t = T_2. \end{cases} \tag{3.20}$$

Verification of (3.2) and (3.3) The values in (3.20) are so small that $\sum_{n=1}^3 C_n(t) D_n(\tau)$ determines the sign of $p(1, t, \tau)$. We obtain

$$\sum_{n=1}^3 C_n(t) D_n(\tau) \begin{cases} < -2.4583e - 04, & \tau = \tau_1, t = \tau_1, \\ > 1.6444e - 05, & \tau = \tau_1, t = T_2, \\ < -5.6792e - 05, & \tau = \tau_2, t = T_1, \\ > 5.6764e - 05, & \tau = \tau_2, t = \tau_2. \end{cases}$$

In view of (3.20), this shows

$$p(1, \tau_1, \tau_1) < 0, \quad p(1, T_2, \tau_1) > 0, \quad p(1, T_1, \tau_2) < 0 \quad \text{and} \quad p(1, \tau_2, \tau_2) > 0.$$

Since $p(1, \cdot, \cdot)$ is continuous on $D := (T_1, T_2) \times [\tau_1, \tau_2]$ there exists at least one root $t(\tau_i)$ for $p(1, \cdot, \tau_i), i = 1, 2$.

In the sequel we will use several times that

$$\begin{aligned} D_1(\tau_1), D_3(\tau_1) < 0 \quad \text{and} \quad D_2(\tau_1) > 0, \\ D_1(\tau_2), D_3(\tau_2) < 0 \quad \text{and} \quad D_2(\tau_2) > 0. \end{aligned} \tag{3.21}$$

Verification of (3.4) and (3.5) The property $\frac{\partial}{\partial \tau} p(1, t, \tau) > 0 \forall (t, \tau) \in (0, T)^2$ is obvious. To obtain $\frac{\partial}{\partial t} p(1, t, \tau) = \sum_{n=1}^{\infty} C'_n(t) D_n(\tau) > 0 \forall (t, \tau) \in D$, it suffices to show it for $\tau = \tau_1$ and every $t \in (T_1, T_2)$, since $\frac{\partial}{\partial t} p(1, t, \cdot)$ is monotone with respect to τ .

For $C'_n(t), n \geq 4$, an analogue of the estimate (3.16) is given by

$$C'_n(t) = \frac{\cos^2(\mu_n)}{N_n} e^{-\mu_n^2(T-t)} \leq 2e^{-(n-1)^2\pi^2(T-t)} \leq 2(e^{-3\pi^2(T-t)})^{n-1} = 2q_T^{n-1},$$

with the above notation. As in (3.19), with the help of (3.20) and (3.21), we deduce by some numerical calculations

$$\sum_{n=4}^{\infty} C'_n(t) |D_n(\tau)| \leq \sum_{n=4}^{\infty} C'_n(T_2) |D_n(\tau)| \leq 2.26 \cdot 10^{-2} \cdot \sum_{n=3}^{\infty} q_{T_2}^n < 10^{-7}$$

and

$$\begin{aligned} \sum_{n=1}^3 C'_n(t) D_n(\tau_1) &\geq C'_1(T_2) \cdot \underbrace{D_1(\tau_1)}_{<0} + C'_2(T_1) \cdot \underbrace{D_2(\tau_1)}_{>0} + C'_3(T_2) \cdot \underbrace{D_3(\tau_1)}_{<0} \\ &> 0.4799026 \cdot (-6.573986 \cdot 10^{-4}) + 0.0197722 \cdot 0.01994057 \\ &\quad + 0.002518234 \cdot (-0.0240712) \\ &> 10^{-5}. \end{aligned}$$

Thus $\frac{\partial}{\partial t} p(1, t, \tau) > 0, \forall (t, \tau) \in D$, implying immediately the uniqueness of $t(\tau_i)$ in $[T_1, T_2]$. Therefore, (3.4), (3.5) are verified. Notice that in all of our numerical values the rounding w.r. to the last digit can be neglected, since it does not change the sign.

Uniqueness of $t(\tau_i), i = 1, 2$ The only assumption of Theorem 3.1 left to be verified is to make sure that $t(\tau_i), i = 1, 2$ are unique in $[0, T]$. To this aim, we next prove that the functions $p(1, \cdot, \tau_i)$ do not have any roots on $[0, T_1) \cup (T_2, T]$, i.e. $p(1, t, \tau_i) < 0, \forall t \in [0, T_1)$ and $p(1, t, \tau_i) > 0, \forall t \in (T_2, T], i = 1, 2$. Because of $\frac{\partial}{\partial \tau} p(1, \cdot, \cdot) > 0$ on $(0, T)^2$ it suffices to show that $p(1, t, \tau_2) < 0 \forall t \in [0, T_1)$ and $p(1, t, \tau_1) > 0 \forall t \in (T_2, T]$. The first inequality is easy to show, since $C_n(t)$ converges very fast when $n \rightarrow \infty$ and t is far from T . For the second one we need to perform a partition of $(T_2, T]$ in appropriate sub-intervals, where we can use the above techniques.

Verification of $p(1, t, \tau_2) < 0, \forall t \in [0, T_1]$: From (3.19) and (3.20), along with the monotonicity of C_n , we deduce

$$\sum_{n=4}^{\infty} C_n(t)|D_n(\tau_2)| \leq c_0 \sum_{n=3}^{\infty} q_{T_1}^n < 10^{-15},$$

where again $c_0 = \frac{2.26}{9\pi^2} \cdot 10^{-2}$. With (3.21), we get

$$\begin{aligned} \sum_{n=1}^3 C_n(t)D_n(\tau_2) &\leq C_1(0) \cdot \underbrace{D_1(\tau_2)}_{<0} + C_2(T_1) \cdot \underbrace{D_2(\tau_2)}_{>0} + C_3(0) \cdot \underbrace{D_3(\tau_2)}_{<0} \\ &< 0.2266498 \cdot (-1.655819 \cdot 10^{-4}) + 0.001685 \cdot 0.020435335 \\ &\quad + 1.6922 \cdot 10^{-30} \cdot (-0.02407) \\ &< -10^{-7}. \end{aligned}$$

Verification of $p(1, t, \tau_1) > 0, \forall t \in (T_2, T]$ For t close to the final time T , higher indexed terms of the series (3.14) becomes relevant, making the above estimations difficult for $t = T$. Next we split $(T_2, T]$ into the following parts: $(T_2, 1.5)$, $[1.5, 1.55]$, $(1.55, 1.57]$ and $(1.57, T]$. We present here only the estimation for the most difficult case $t \in (1.57, T]$. The intervals $(T_2, 1.5)$, $[1.5, 1.55]$ and $(1.55, 1.57]$ are discussed for completeness in the Appendix.

Case $t \in (1.57, T]$: Here $q_T = 1$, hence the only rapidly converging term is μ_n^{-2} . On $(1.57, T]$, we have

$$\begin{aligned} \sum_{n=4}^{\infty} C_n(t)|D_n(\tau_1)| &\leq \sum_{n=4}^{\infty} C_n(T)|D_n(\tau_1)| \leq 1.13 \cdot 10^{-2} \cdot \sum_{n=4}^{\infty} \frac{2}{\mu_n^2} \\ &\leq 2.26 \cdot 10^{-2} \cdot \sum_{n=4}^{\infty} \frac{1}{\pi^2(n-1)^2} \leq \frac{2.26 \cdot 10^{-2}}{\pi^2} \cdot \left[\frac{\pi^2}{6} - 1 - \frac{1}{4} \right] \\ &< 9.04343 \cdot 10^{-4}, \end{aligned}$$

while

$$\begin{aligned} \sum_{n=1}^3 C_n(t)D_n(\tau_1) &\geq C_1(T) \cdot \underbrace{D_1(\tau_1)}_{<0} + C_2(1.57) \cdot \underbrace{D_2(\tau_1)}_{>0} + C_3(T) \cdot \underbrace{D_3(\tau_1)}_{<0} \\ &> 0.7298807 \cdot (-6.573986 \cdot 10^{-4}) + 0.12949167 \cdot 0.01994057 \\ &\quad + 0.04604178 \cdot (-0.0240712) \\ &> 9.94034 \cdot 10^{-4}. \end{aligned}$$

Thus it holds

$$p(1, t, \tau_1) > 9.94034 \cdot 10^{-4} - 9.04343 \cdot 10^{-4} > 0 \quad \forall t \in (1.57, T].$$

Altogether, $p(1, t, \tau_2) < 0 \forall t \in [0, T_1]$ and $p(1, t, \tau_1) > 0 \forall t \in (T_2, T]$. Thanks to these facts and to the estimations in the Appendix, we are able to prove the following result:

Theorem 3.4 *With $\alpha = 1$, $T = 1.58$ and $y_d = (1 - x^2)/2$, the Robin boundary control problem (\mathcal{P}_α) admits a unique optimal control \bar{u} which is bang-bang and has a single switching point $\bar{\tau}$ in $[1.329, 1.3294]$.*

Proof In the estimations above, we have shown that there exists an optimal control \bar{u} having the bang-bang property stated in the theorem. It remains to show its uniqueness. This holds true, if the optimal value associated with \bar{u} is positive. In that case, the theory yields that any optimal control must be bang-bang, and this ensures uniqueness. Therefore, we verify that the corresponding functional value is not zero. We prove the existence of an interval $E \subset [0, 1]$ with positive measure, such that

$$|y(x, T) - y_d(x)| \neq 0, \tag{3.22}$$

for every $x \in E$. Since $\bar{y}(\cdot, T)$ and y_d are continuous, it suffices to verify (3.22) for a single $x \in [0, 1]$. At $x = 1$, it holds $y_d(1) = 0$ and from (3.10)

$$\bar{y}(1, T) = \sum_{n=1}^{\infty} \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) [2e^{-\mu_n^2(T-\bar{\tau})} - e^{-\mu_n^2 T}] - 1.$$

Obviously, all terms $\frac{1}{N_n \mu_n^2} \cos^2(\mu_n) [2e^{-\mu_n^2(T-\bar{\tau})} - e^{-\mu_n^2 T}]$ are nonnegative, therefore it is enough to evaluate numerically as many terms of the series until their sum exceeds 1. In our case we may stop this procedure after the first two terms, since

$$\begin{aligned} & \sum_{n=1}^2 \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) [2e^{-\mu_n^2(T-\bar{\tau})} - e^{-\mu_n^2 T}] \\ & \geq \sum_{n=1}^2 \frac{1}{N_n \mu_n^2} \cos^2(\mu_n) [2e^{-\mu_n^2(T-1.329)} - e^{-\mu_n^2 T}] > 1.00092. \end{aligned} \quad \square$$

The issue discussed above is very sensitive with respect to α . To our surprise, the case $\alpha > 1$ exhibited a completely different behaviour compared to what we studied up to now. The left part of Fig. 5 shows the optimal control of the problem (P_α) , $\frac{1}{\alpha} = 0.99$, attained numerically by a primal-dual active set strategy on a grid with $n_x = 101$ equidistant points in the spatial domain $[0, 1]$ and $n_t = 101$ equidistant points in the time domain $[0, T]$ for the control discretization. We underline again that all other numerical computations are based on the Fourier method. Obviously, this control does not sufficiently well satisfy (2.9) in the vicinity of T ; cf. the right part of Fig. 5.

We investigate the behaviour with respect to α in Sect. 6.

Example 3 We take all data as in Example 2 except y_d , which is defined by $y_d(x) = \frac{1}{2}(1 - x)$.

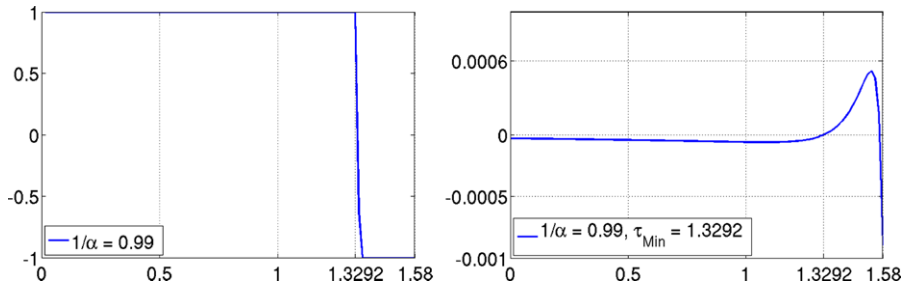


Fig. 5 $\frac{1}{\alpha} = 0.99, N = 5, n_x = n_t = 101, \tau_{Min} = \bar{\tau}; \bar{u}$ and $p(1, \cdot, \tau_{Min})$

This example shows that one cannot really trust in numerical results only. A numerical computation with fairly small grid delivers also a bang-bang solution with one switching point. Refining the grid considerably, more switching points appear. We think that many switching points exist in this second example, cf. [3].

4 Reduction to moment problems

Here, we study the attainability of y_d by a theoretical tool, the well known exponential moment problem whose relevance to boundary control problems for the heat equation has been extensively studied (see Gal'chuk [8], Fattorini and Russell [7], Schmidt [21], Krabs [11]). By reducing the control problems (\mathcal{P}_N) and (\mathcal{P}_α) to certain exponential moment problems, we derive some useful necessary conditions for restricted reachability.

4.1 Known results on reachability

Let $\{\lambda_n\}_{n \in \mathbb{N}}$ be a strictly increasing, unbounded sequence of positive real numbers, satisfying

$$\sum_{n=0}^{\infty} \frac{1}{\lambda_n} < \infty. \tag{4.1}$$

Given $T \in (0, \infty]$ and a sequence $\{c_n\}_{n \in \mathbb{N}}, c_n \in \mathbb{R}$, not all equal to zero, the *exponential moment problem* consists of finding a function $u \in L^\infty(0, T)$, such that

$$\int_0^T u(t)e^{-\lambda_i t} dt = c_i \quad \text{for each } i \in \mathbb{N}. \tag{4.2}$$

The *problem of reachability* of y_d , subject to the PDE (1.2), can be formulated in terms of a exponential moment problem. Let a terminal condition

$$y(\cdot, T) = y_d \in L^2(0, 1) \tag{4.3}$$

be given. The question is, whether there exists a boundary control, such that the solution of the state equation (1.2) also satisfies (4.3). Note that the above formulation of the moment problem does not yet include the restriction (1.3).

Let us consider a more general case of the state equations (1.2), where additionally an initial temperature distribution $y(\cdot, 0) = y_0 \in L^2(0, 1)$ is given. Define the *set of reachable states*

$$R_T(y_0, L^\infty) := \{y(\cdot, T) \mid \exists u \in L^\infty(0, T) \text{ with } y = y(u), \text{ where } y(\cdot, 0) = y_0, \\ y(u) \text{ denotes the corresponding solution of (1.2)}\}.$$

A necessary and sufficient condition for solving the moment problem (4.2) is given in [18]. As a consequence of it we have

Proposition 4.1 ([12]) *The moment problem (4.2) is solvable if the sequence $\{c_n\}_{n \in \mathbb{N}}$ is given by*

$$c_j = \sum_{k=0}^N a_k \lambda_j^{-k},$$

for some $N \in \mathbb{N}$ and $a_1, \dots, a_N \in \mathbb{R}$.

Sufficient conditions for the reachability of an arbitrary y_d by optimal controls of the Dirichlet problem are discussed in [17] (see also [5]).

It is well known that $R_T(y_0, L^\infty)$ is dense in $L^2(0, 1)$ (see [14]), that $0 \in R_T(y_0, L^\infty)$ (a property known as null-controllability, see [17]) and that $R_T(y_0, L^\infty)$ is in fact independent of T and y_0 (see [4]).

Proposition 4.2 (see [18, Corollary 4]) *For the Dirichlet and Robin boundary problem, every polynomial belongs to $R_T(0, L^\infty) \forall T > 0$.*

Thus, for arbitrary, but fixed $T > 0$ there exists $\bar{u} \in L^\infty(0, T)$, not necessarily satisfying the control constraints (1.3), whose final state $\bar{y}(\cdot, T)$ coincides with y_d , i.e. $J(\bar{y}, \bar{u}) = 0$. Since the *countable bang-bang principle* (Theorem 2.3) does not hold in this case, the uniqueness of \bar{u} is not granted.

Remark 4.3 Due to the regularizing effect of the heat equation, in the case of Neumann or Dirichlet boundary conditions, reachable states are real-analytic, cf. [6, 7].

Notice that also the problem of null controllability falls into this class. If y_0 is a non-zero initial state, then the solution y at time $t = T$ can be written as

$$y(\cdot, T) = (Su) + (S_0 y_0)(\cdot, T),$$

where S_0 is the mapping $y_0 \mapsto y(\cdot, T)$ for $u = 0$. Therefore, the problem to reach $y(\cdot, T) = 0$ is covered by our problem for

$$y_d = -(S_0 y_0)(\cdot, T).$$

Clearly, this y_d is very smooth. For results on null-controllability we refer to Fattorini and Russell [7] and Gal'chuk [8].

However, also these results do not contain precise information on the $L^\infty(0, T)$ -norm of the controls needed to reach the target y_d , no matter how smooth it is.

Higher smoothness of y_d , in particular of $S_0 y_0$ in the case of null controllability, does not yield an easier numerical confirmation. For instance, it would be interesting to know, for which classes of target states the number of switching points of the optimal bang-bang control is finite, if y_d is not reachable under the given control restrictions. We do not have an answer to this question. For instance, think of the function $y_d(x) = \frac{1}{2}(1 - x)$ mentioned in Example 3.

4.2 Restricted reachability by Neumann boundary controls

In order to reduce the control problem to a moment problem, we first expand $y_d(x) = (1 - x^2)/2$ in a Fourier series,

$$y_d(x) = a_0 + \sum_{n=1}^\infty a_n \cos(n\pi x), \quad a_n = \begin{cases} 2 \int_0^1 y_d(\xi) \cos(n\pi \xi) d\xi, & n > 0, \\ \int_0^1 y_d(\xi) d\xi, & n = 0. \end{cases}$$

We obtain $a_0 = 1/3$ and, for $n > 0$,

$$a_n = \int_0^1 (1 - x^2) \cos(n\pi x) dx = (-1)^{n+1} \frac{2}{n^2 \pi^2}.$$

Thus it holds

$$y_d(x) = \frac{1}{3} - 2 \sum_{n=0}^\infty \frac{(-1)^n}{n^2 \pi^2} \cos(n\pi x), \quad x \in [0, 1]. \tag{4.4}$$

By comparing the coefficients of

$$y(x, T) = (Su)(x) = \int_0^T \left[1 + 2 \sum_{n=1}^\infty (-1)^n \cos(n\pi x) e^{-n^2 \pi^2 (T-s)} \right] u(s) ds$$

with those of (4.4), the problem of reachability (4.3) can be formulated in terms of the solvability of the following infinite system of equations:

$$\begin{cases} \int_0^T u(s) ds = \frac{1}{3}, \\ \int_0^T e^{-n^2 \pi^2 (T-s)} u(s) ds = -\frac{1}{n^2 \pi^2}, \quad n > 0. \end{cases} \tag{4.5}$$

To generalize (1.3), we consider controls with values contained in $[-c, c]$, $c > 0$, and derive a necessary condition for restricted reachability depending on T and c .

In order to circumpass difficulties with signs, we perform the transformation $v(t) := \frac{1}{2}(u(t) + c)$. Then $|u(t)| \leq c$ is equal to $v(t) \in [0, c]$. From (4.5) we deduce

$$\int_0^T v(s) ds = \frac{1}{2}cT + \frac{1}{6}, \tag{4.6}$$

$$\int_0^T e^{-n^2 \pi^2 (T-s)} v(s) ds = \frac{1}{2n^2 \pi^2} [c - 1 - ce^{-n^2 \pi^2 T}], \quad n > 0. \tag{4.7}$$

Lemma 4.4 *The conditions*

$$cT \geq \frac{1}{3} \quad \text{and} \quad c - 1 - ce^{-n^2\pi^2T} \geq 0 \quad \forall n > 0$$

are necessary for restricted reachability of y_d by Neumann boundary controls.

Proof Since $v(t) \leq c$, it follows that $\int_0^T v(s) ds \leq cT$, hence from (4.6)

$$\frac{1}{2}cT + \frac{1}{6} \leq cT, \quad \text{i.e.} \quad \frac{1}{3} \leq cT.$$

Because of $v(t) \geq 0$ we deduce from (4.7) that $0 \leq c - 1 - ce^{-n^2\pi^2T} \forall n > 0$. □

The next theorem follows instantly from the second inequality of Lemma 4.4.

Theorem 4.5 *For all $c \in [0, 1]$, $y_d(x) = (1 - x^2)/2$, $x \in [0, 1]$, is not reachable by any Neumann boundary control u with $|u(t)| \leq c$ at any time $T > 0$.*

For $c > 1$ we deduce the necessary condition

$$c[1 - e^{-n^2\pi^2T}] \geq 1, \quad \text{that is} \quad e^{-n^2\pi^2T} \leq 1 - \frac{1}{c},$$

which has to be satisfied in particular for $n = 1$. Hence it must hold:

$$T \geq -\frac{1}{\pi^2} \ln\left(1 - \frac{1}{c}\right).$$

4.3 Restricted reachability by Robin boundary controls

By the Fourier series expansion of y_d , we get with the notation of Sect. 2

$$y_d(x) = \sum_{n=1}^{\infty} b_n v_n(x), \quad b_n = \frac{1}{2\sqrt{N_n}} \int_0^1 \cos(\mu_n x)(1 - x^2) dx$$

and from (3.12) we find

$$y_d(x) = \sum_{n=1}^{\infty} \frac{1}{N_n} \cos(\mu_n x) \left[\frac{\sin(\mu_n)}{\mu_n^3} - \frac{\cos(\mu_n)}{\mu_n^2} \right]. \tag{4.8}$$

Similarly to the previous subsection, the problem of reachability can therefore be expressed by

$$\int_0^T e^{-\mu_n^2(T-s)} u(s) ds = \frac{1}{\mu_n^4} - \frac{1}{\alpha\mu_n^2}, \quad \text{for all } n = 1, 2, \dots$$

The unrestricted reachability of y_d , for every $T > 0$ is then an immediate consequence of Proposition 4.1 ($N = 4$, $a_0 = a_1 = a_3 = 0$, $a_2 = -1/\alpha$, $a_4 = 1$) (see also

Proposition 4.2). Let us now assume again $|u(t)| \leq c, c > 0$. Transforming again u into $v, v(t) \in [0, c]$, by $v(t) = \frac{1}{2}(u(t) + c), t \in [0, T]$, we get

$$\int_0^T e^{-\mu_n^2(T-s)} [2v(s) - c] ds = \frac{1}{\mu_n^4} - \frac{1}{\alpha \mu_n^2}. \tag{4.9}$$

Consequently, we have the following

Theorem 4.6 *The condition*

$$c[1 - e^{-\mu_n^2 T}] \geq \left| \frac{1}{\mu_n^2} - \frac{1}{\alpha} \right| \quad \forall n = 1, 2, \dots \tag{4.10}$$

is necessary for restricted reachability of y_d by Robin boundary controls.

Proof Because of $v(t) \geq 0$ and $v(t) \leq c$ it follows from (4.9)

$$c[1 - e^{-\mu_n^2 T}] \geq -\left[\frac{1}{\mu_n^2} - \frac{1}{\alpha} \right] \quad \text{and} \quad c[1 - e^{-\mu_n^2 T}] \geq \frac{1}{\mu_n^2} - \frac{1}{\alpha},$$

respectively, thus (4.10) follows immediately. □

The inequality (4.10) can also be deduced from the general inequality (A.3) in Schmidt [21].

Considering again our Example 2 ($T = 1.58, c = \alpha = 1$) the inequality (4.10) is satisfied for every $n \geq 1$. This shows that the necessary condition (4.10) is not sufficient for the reachability of y_d by admissible Robin boundary controls.

For the case $T = 1.58, \alpha < 1$ and $c = 1$, the condition (4.10) is not satisfied because $\mu_n \rightarrow \infty$ as $n \rightarrow \infty$ and therefore, passing to the limit in (4.10) yields $1 \geq \frac{1}{\alpha}$ which is not true.

Conclusion 4.7 *For $\alpha < 1, T = 1.58$ and $y_d(x) = \frac{1}{2}(1 - x^2)$, is not reachable by Robin boundary controls that satisfy (1.3).*

Based on these results we have the impression that $\alpha = 1$ is the limit value, which separates the optimal control problems (P_α) , where $y_d(x) = \frac{1}{2}(1 - x^2)$ is attainable from those where y_d is not, i.e. for $\alpha > 1$ there exists an admissible control such that the solution of the state equation (1.2) also satisfies (4.3), cf. our numerical results in Sect. 6.

5 Optimal controls with two switching points

The method of Theorem 3.1 can be extended to controls with more than one switching point. For two switching points, we have a similar result at our disposal, where the first switching point τ_1 has to be found yet, while we assume that a second switching point $\tau_2 = \tau_2(\tau_1)$ exists that coincides with a zero of $p(1, t)$ (for all τ_1 out of a

certain interval). With respect to τ_1 , the theory is analogous to the case of one switching point. However, we found it difficult to apply this result. Instead, we present an application of a theorem by Miranda [15].

We shall investigate the problem (\mathcal{P}_N) in the case, where the optimal control u^* is bang-bang and has exactly two switching points $\tau_1, \tau_2 \in (0, T)$, denoted by τ_1^*, τ_2^* . Here, we use the star to avoid notational confusion in the next examples. We assume that u^* belongs to the class of controls that have the form

$$u(t) = u(t, \tau_1, \tau_2) = \begin{cases} -1, & t \in (0, \tau_1) \cup (\tau_2, T), \\ 1, & t \in (\tau_1, \tau_2), \end{cases} \tag{5.1}$$

where $\tau_1 < \tau_2$.

First, we introduce some necessary notation. We define the faces of the open cube $Q(x^0, \rho)$ in $\mathbb{R}^n, n \geq 1$, centered at x^0 with side length $2\rho, \rho > 0$,

$$Q_+^i(x^0, \rho) = \{x \in Q(x^0, \rho) \mid x_i - x_i^0 = \rho\},$$

$$Q_-^i(x^0, \rho) = \{x \in Q(x^0, \rho) \mid x_i - x_i^0 = -\rho\}.$$

Then Miranda’s theorem can be stated as follows:

Theorem 5.1 ([15]) *Let $f : \mathbb{R}^n \supseteq \overline{Q(x^0, \rho)} \rightarrow \mathbb{R}^n$ be a continuous mapping. Assume that*

$$f_i(x) \begin{cases} \geq 0 & \text{for all } x \in Q_+^i(x^0, \rho), \\ \leq 0 & \text{for all } x \in Q_-^i(x^0, \rho) \end{cases}$$

holds for all $i = 1, \dots, n$. Then f has at least one zero in $\overline{Q(x^0, \rho)}$.

The following extension of Miranda’s theorem to rectangles was proven in [19].

Corollary 5.2 *Assume that $x^0 \in \mathbb{R}^n$ and numbers $L_i \geq 0$, for $i = 1, \dots, n$ be given. Let $R \subset \mathbb{R}^n$ be the rectangle $R = \{x \in \mathbb{R}^n \mid |x_i - x_i^0| \leq L_i, i = 1, \dots, n\}$ and $f : R \rightarrow \mathbb{R}^n$ a continuous mapping on R . Define the pairs of parallel opposite faces of the rectangle R by*

$$R_+^i := \{x \in R \mid x_i = x_i^0 + L_i\}, \quad R_-^i := \{x \in R \mid x_i = x_i^0 - L_i\}, \quad i = 1, \dots, n.$$

If

$$f_i(x) \cdot f_i(y) \leq 0, \quad \forall x \in R_+^i, y \in R_-^i,$$

holds for all $i = 1, \dots, n$, then there exists some $\bar{x} \in R$ satisfying $f(\bar{x}) = 0$.

On the basis of this result, we now discuss optimal control problems, where the optimal control u^* is bang-bang with exactly two switching points. For simplicity, we discuss only the problem with Neumann boundary control.

Analogously to (3.7), we obtain for a control function u having the form (5.1) that

$$S^*Su(t, \tau_1, \tau_2) = 2(\tau_2 - \tau_1) - T + 2 \sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} e^{-n^2\pi^2(T-t)} \times [2(e^{-n^2\pi^2(T-\tau_2)} - e^{-n^2\pi^2(T-\tau_1)}) - e^{-n^2\pi^2T}]. \tag{5.2}$$

First, we construct an example in an explicit analytical way. Next, we slightly perturb the data to show how the theorem of Miranda can be applied to confirm the existence of an optimal bang-bang control with two switching points. To construct the analytical example, first we choose a function $w \neq 0$ such that S^*w has exactly two roots $\tau_1^*, \tau_2^* \in (0, T)$. This function w stands for $Su^* - y_d$. Next, we just define $u^* := u(\cdot, \tau_1^*, \tau_2^*)$ which satisfies the sign condition, $\text{sign } S^*w(t) = 1$ on $[0, \tau_1^*]$, and we fix $y_d := Su^* - w$. Then u^* satisfies the necessary optimality condition and is optimal. Let us proceed in this way.

Example 4 We take $T = 1, w(x) = x^2 - \frac{5}{4}x + \frac{3}{10}$. The roots τ_1^*, τ_2^* of

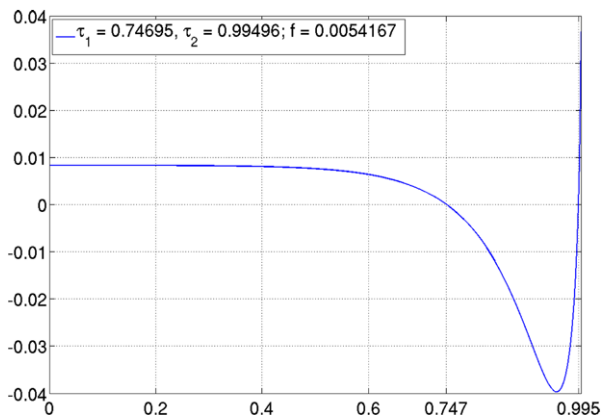
$$\begin{aligned} (S^*w)(t) &= \int_0^1 \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n \cos(n\pi\xi) e^{-n^2\pi^2(T-t)} \right] w(\xi) d\xi \\ &= \frac{1}{120} + \frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{n^2\pi^2} e^{-n^2\pi^2(T-t)} [5(-1)^n + 3] \end{aligned}$$

are approximately located at $\hat{\tau}_1 := 0.74695$ and $\hat{\tau}_2 := 0.99496$. As previously mentioned, we set $u^* := u(\cdot, \tau_1^*, \tau_2^*)$ and $y_d := Su^* - w$.

In this example, we know the optimal control exactly. However, from a numerical point of view this is not entirely true, because we obtain only (very good) approximations $\hat{\tau}_1, \hat{\tau}_2$ of the switching points.

Since the series for S^*w converges very slowly close to T , other zeros S^*w than τ_1^* and τ_2^* might be hidden at the end of $[0, T]$. We have to exclude this possibility. The graph of S^*w is shown in Fig. 6, and it is obvious due to the precision of

Fig. 6 S^*w computed for $n_x = n_t = 1001$ and $N = 100$; $f = J(\bar{y}, \bar{u})$



our computations with Fourier series that another zero can only exist in $[0.99, 1]$. It suffices to prove that S^*w is strictly monotone increasing in the interval $(0.99, 1)$. Therefore, we verify that the derivative of S^*w ,

$$(S^*w)'(t) = \frac{1}{2} \sum_{n=1}^{\infty} e^{-n^2\pi^2(T-t)} [5(-1)^n + 3], \tag{5.3}$$

is strictly positive for every $t \in (0.99, T)$. By splitting the series (5.3) into the part of odd and even items, we get after an index shift in the odd part

$$\begin{aligned} (S^*w)'(t) &= 4 \sum_{n=1}^{\infty} e^{-4n^2\pi^2(T-t)} - e^{-\pi^2(T-t)} \sum_{n=1}^{\infty} e^{-4n(n+1)\pi^2(T-t)} - e^{-\pi^2(T-t)} \\ &\geq (4 - e^{-\pi^2(T-t)}) \sum_{n=1}^{\infty} e^{-4n^2\pi^2(T-t)} - e^{-\pi^2(T-t)} \\ &> 3e^{-4\pi^2(T-t)} - e^{-\pi^2(T-t)} = e^{-\pi^2(T-t)} \{3e^{-3\pi^2(T-t)} - 1\}. \end{aligned}$$

In $[0.99, 1]$, the term in braces can be estimated from below by $3e^{-\frac{3}{100}\pi^2} - 1 > 1.23$, hence S^*w is monotone increasing in $(0.99, 1)$.

Let us now slightly change the situation. We construct a related example, where we do not know the exact optimal control but a very good approximation. Then we confirm by Corollary 5.2 that the optimal control has exactly two switching points in a prescribed region.

Example 5 We take w as in Example 4 (notice that S^*w has exactly the roots τ_1^*, τ_2^*) and define an auxiliary control \hat{u} by

$$\hat{u}(t) = u(t, \hat{\tau}_1, \hat{\tau}_2) = \begin{cases} -1, & t \in (0, \hat{\tau}_1) \cup (\hat{\tau}_2, T), \\ 1, & t \in (\hat{\tau}_1, \hat{\tau}_2), \end{cases}$$

where $\hat{\tau}_1 = 0.74695$ and $\hat{\tau}_2 = 0.99496$ are the numerical approximations of τ_1^*, τ_2^* . Moreover, we fix $y_d := S\hat{u} - w$. Then $w = S\hat{u} - y_d$, and $S^*w = S^*(S\hat{u} - y_d)$ has roots different from τ_i^* and $\hat{\tau}_i, i = 1, 2$, hence \hat{u} is not optimal for this problem. Also u^* is not optimal. We find

$$\begin{aligned} y_d(x) &= (S\hat{u})(x) - w(x) \\ &= 2(\hat{\tau}_2 - \hat{\tau}_1) - T - \frac{3}{2}x^2 + \frac{5}{4}x - \frac{2}{15} \\ &\quad + 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2\pi^2} \cos(n\pi x) [2(e^{-n^2\pi^2(T-\hat{\tau}_2)} - e^{-n^2\pi^2(T-\hat{\tau}_1)}) + e^{-n^2\pi^2T}]. \end{aligned} \tag{5.4}$$

Now, our goal is to confirm that this problem has an optimal bang-bang control \hat{u} of the form (5.1). Along with (5.2), we have for a control u with two switching

points τ_1, τ_2 ,

$$\begin{aligned}
 p(1, t, \tau_1, \tau_2) &= S^*(Su(\tau_1, \tau_2) - y_d)(t) \\
 &= S^*(Su(\tau_1, \tau_2) - (S\hat{u} - w))(t) \\
 &= 2(\tau_2 - \tau_1) - 2(\hat{\tau}_2 - \hat{\tau}_1) + \frac{1}{120} \\
 &\quad + 2 \sum_{n=1}^{\infty} \frac{1}{n^2 \pi^2} e^{-n^2 \pi^2 (T-t)} \left[2(e^{-n^2 \pi^2 (T-\tau_2)} - e^{-n^2 \pi^2 (T-\tau_1)}) \right. \\
 &\quad \left. - 2(e^{-n^2 \pi^2 (T-\hat{\tau}_2)} - e^{-n^2 \pi^2 (T-\hat{\tau}_1)}) + \frac{5}{4}(-1)^n + \frac{3}{4} \right]. \tag{5.5}
 \end{aligned}$$

To calculate the functional value of a control of the form (5.1) we have to solve the differential equation (1.2) numerically. For that purpose we use a standard central difference approximation of the Laplace operator and an implicit Euler scheme for the time integration. In order to achieve a good quality of the numerical approximation of our example, we used a finer discretisation of the space and time interval than that used in Sect. 3.

As in the preceding sections, n_x and n_t stand for the discretization in space and time used for evaluating all integrals by the trapezoidal rule, while N is the termination index for the Fourier series. Taking $n_x = 1001$ we can reduce the difference between the functional value of $u(\cdot, \hat{\tau}_1, \hat{\tau}_2)$ and $\frac{1}{2} \int_0^1 (w(x))^2 dx = \frac{13}{2400}$ to the range of 10^{-6} . Note that $\frac{1}{2} \int_0^1 (w(x))^2 dx$ is the optimal value of Example 4. Moreover, since $\hat{\tau}_2$ is very close to the final time T , a smaller grid parameter $\tau = 1/(n_t - 1)$ with respect to time is needed. Figure 6 shows the adjoint state $p(1, \cdot, \hat{\tau}_1, \hat{\tau}_2)$ corresponding to \hat{u} when $n_x = n_t = 1001$ and $N = 100$. We underline again that these numerical computations are based on the Fourier method. The necessity to compute the series in (5.5) up to a rather large N , e.g. $N = 100$, is due to the increasing importance of higher indexed items as t tends to T .

5.1 Existence of an optimal bang-bang control via Miranda’s theorem

Let $R := [0.745, 0.749] \times [0.994, 0.996]$ be the rectangle with midpoint $\tau^0 = (\tau_1^0, \tau_2^0) = (0.747, 0.995)$ and side lengths $L_1 = 2 \cdot 10^{-3}$ and $L_2 = 1 \cdot 10^{-3}$.

We assume that for every pair of switching points $(\tau_1, \tau_2) \in R$, the function $p(1, \cdot, \tau_1, \tau_2)$, associated with the bang-bang control $u(\cdot, \tau_1, \tau_2)$ of the form (5.1), has exactly two roots denoted by $0 < t_1(\tau_1, \tau_2) < t_2(\tau_1, \tau_2) < T$. By Miranda’s theorem, we confirm the existence of a fixed point of the mapping $(\tau_1, \tau_2) \mapsto (t_1(\tau_1, \tau_2), t_2(\tau_1, \tau_2))$ or, equivalently, the existence of a root for

$$f : \mathbb{R}^2 \supset R \rightarrow \mathbb{R}^2, \quad f(\tau_1, \tau_2) = \begin{bmatrix} f_1(\tau_1, \tau_2) \\ f_2(\tau_1, \tau_2) \end{bmatrix} := \begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix} - \begin{bmatrix} t_1(\tau_1, \tau_2) \\ t_2(\tau_1, \tau_2) \end{bmatrix}. \tag{5.6}$$

Fig. 7 4 possible cases for the roots of $p(1) = p(1, \cdot, \tau_1, \tau_2)$

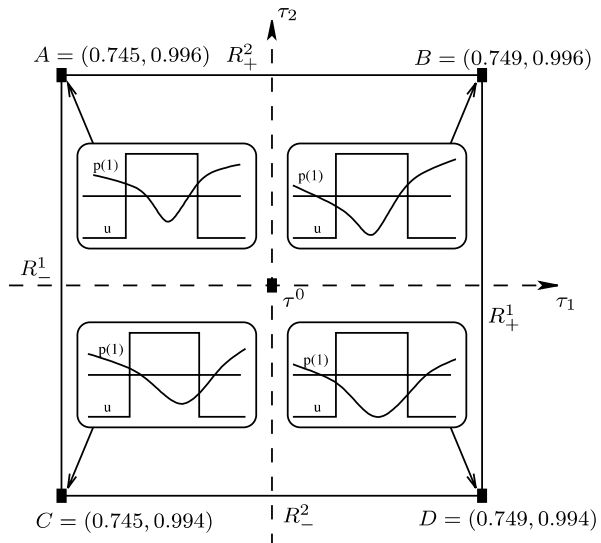


Figure 7 illustrates the situation at the boundary points $A = (0.745, 0.996)$, $B = (0.749, 0.996)$, $C = (0.745, 0.994)$, and $D = (0.749, 0.994)$, of the faces R_{\pm}^i , $i = 1, 2$. Moving along the north edge R_+^2 from B to A , we observe that $f_2 > 0$, while f_1 changes its sign. On the other hand, moving along the west edge R_-^1 from A to C , there holds $f_1 < 0$, but f_2 changes its sign. An analogous behaviour is observed on R_-^2 and R_+^1 . Notice that here we do not prove these inequalities by careful estimations as in the last sections, because this is fairly tedious. Therefore, we do not really *prove* the next results, although this should be possible on the basis of exact estimations. We just take them for granted by our numerical computations.

Figure 8 shows the locations of the roots of $p(1, \cdot, \tau_1, \tau_2)$ subject to the switching points, when (τ_1, τ_2) are the points A, B, C, D . A study of Fig. 7 reveals that, at the corner B , the zeros t_i of $p(1, \cdot)$ are located left of τ_i , $i = 1, 2$. Therefore, $f_1(B) > 0$ and $f_2(B) > 0$. Similarly, we have $f_1(C) < 0$ and $f_2(C) < 0$.

To apply Corollary 5.2, we need to know the signs of f_i , $i = 1, 2$, in every point of the faces R_{\pm}^i . The following assumption will make this easier. The points B and C play a special role in this context.

Assumption 5.3 For every $(\tau_1, \tau_2) \in R$, there holds

$$\frac{\partial p}{\partial t}(1, t_1(\tau_1, \tau_2), \tau_1, \tau_2) < 0 \quad \text{and} \quad \frac{\partial p}{\partial t}(1, t_2(\tau_1, \tau_2), \tau_1, \tau_2) > 0.$$

In our example, this obviously holds in the corner points A, B, C, D , cf. Fig. 8. In the points between, we confirmed this numerically. Also here, we do not perform exact estimations.

Remark 5.4 Under Assumption 5.3 it suffices to investigate f at the boundary points $B = (0.749, 0.996)$ and $C = (0.745, 0.994)$ only. To see this, we argue as follows: From (5.5) it follows easily that $\frac{\partial p}{\partial \tau_1}(1, t, \tau_1, \tau_2) < 0$ and $\frac{\partial p}{\partial \tau_2}(1, t, \tau_1, \tau_2) > 0$

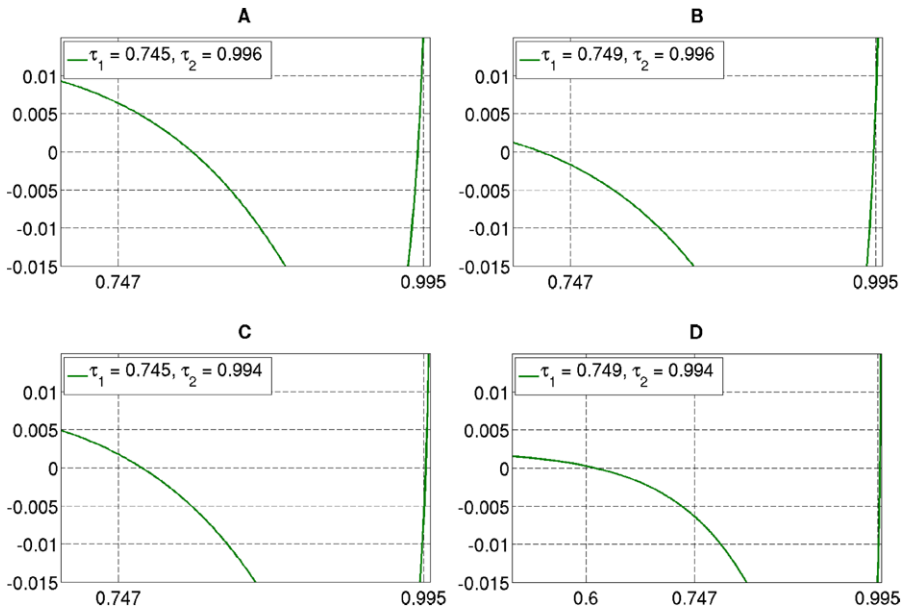


Fig. 8 Details of $p(1, \cdot, \tau_1, \tau_2)$ around the roots when $(\tau_1, \tau_2) \in \{A, B, C, D\}$, $n_t = n_x = 1001$, $N = 100$

$\forall t \in (0, T)$, $(\tau_1, \tau_2) \in \mathbb{R}^2$. In view of our assumption and $p(1, t_i(\tau_1, \tau_2), \tau_1, \tau_2) = 0 \forall (\tau_1, \tau_2) \in R$, the implicit function theorem can be applied as in the proof of Theorem 3.1, hence

$$\frac{\partial t_i}{\partial \tau_j}(\tau_1, \tau_2) = -\frac{\frac{\partial p}{\partial \tau_j}(1, t_i(\tau_1, \tau_2), \tau_1, \tau_2)}{\frac{\partial p}{\partial t}(1, t_i(\tau_1, \tau_2), \tau_1, \tau_2)} > 0, \quad \text{for } i, j \in \{1, 2\}, i \neq j. \quad (5.7)$$

We already know $f_i(B) > 0$ and $f_i(C) < 0$, $i = 1, 2$. Let us take $x = (\tau_1, \tau_2) \in R_+^2$, i.e. $\tau_2 = 0.996$ is fixed and $\tau_1 \leq 0.749$. For $f_2(x) = g(\tau_1) := \tau_2 - t_2(\tau_1, \tau_2)$, it follows from (5.7) that $g'(\tau_1) = -\frac{\partial t_2}{\partial \tau_1}(\tau_1, \tau_2) < 0$, hence $g(\tau_1) \geq f_2(B) > 0 \forall \tau_1 \in [0.745, 0.749]$. In the same way, for $y = (\tau_1, \tau_2) \in R_-^2$, i.e. $\tau_2 = 0.994$ is fixed and $\tau_1 \geq 0.745$, we define $f_2(y) = h(\tau_1) := \tau_2 - t_2(\tau_1, \tau_2)$. Again, from (5.7), we obtain $h'(\tau_1) = -\frac{\partial t_2}{\partial \tau_1}(\tau_1, \tau_2) < 0$ and $f_2(y) = h(\tau_1) \leq f_2(C) < 0 \forall \tau_1 \in [0.745, 0.749]$. Analogously, we show that $f_1(x) > 0$ and $f_1(y) < 0 \forall x \in R_+^1, y \in R_-^1$.

Conclusion 5.5 *Suppose that Assumption 5.3 holds. In our example, we have confirmed this numerically for $T = 1$ and y_d given as in (5.4), where $\hat{\tau}_1 = 0.74695$, $\hat{\tau}_2 = 0.99496$. Then for the problem (\mathcal{P}_N) a bang-bang control \bar{u} with two switching points $\bar{\tau}_1, \bar{\tau}_2$ exists which coincide with the associated zeros of $p(1, \cdot)$.*

Proof Let $\tau^0 = (0.747, 0.995)$, $L_1 = 2 \cdot 10^{-3}$, $L_2 = 1 \cdot 10^{-3}$ and define f as in (5.6). Since $f_i(B) > 0$, $f_i(C) < 0$, for $i = 1, 2$, and taking into account Remark 5.4, we may apply Corollary 5.2 to obtain the existence of $(\bar{\tau}_1, \bar{\tau}_2) \in R$, such that $t_1(\bar{\tau}_1, \bar{\tau}_2) = \bar{\tau}_1$ and $t_2(\bar{\tau}_1, \bar{\tau}_2) = \bar{\tau}_2$. □

The theorem of Miranda ensures the existence of a zero in the rectangle R but does not guarantee its uniqueness. Therefore, a strictly analytical reasoning should exclude other roots in R . Here, we take it for granted by the numerical results, cf. also Fig. 8. The principle shape of these graphs will not change while moving (τ_1, τ_2) through R .

The bang-bang control (5.1), where τ_i is replaced by $\bar{\tau}_i$, $i = 1, 2$, satisfies the optimality condition (2.9), if we verify in addition that the sign of the control equals the negative sign of $p(1, \cdot, \bar{\tau}_1, \bar{\tau}_2)$. In our example, this can be confirmed numerically. Again, we underline that we did not perform the associated estimates to make this a real proof.

The uniqueness is a consequence of the countable bang-bang principle, if we confirm in addition that the minimal value of the objective functional is positive.

6 Application—approximation of Dirichlet boundary controls

As pointed out in the introduction, we were initially interested in approximating the Dirichlet boundary condition by a Robin condition as $\alpha = \beta \rightarrow \infty$. For elliptic Dirichlet boundary control problems, this issue was discussed by Casas et al. [2], who proved convergence and error estimates w.r. to the penalization parameter that corresponds to α . In the control of parabolic PDEs, the optimality conditions for Dirichlet controls can also be achieved by passing to the limit, $\alpha = \beta \rightarrow \infty$, in the optimality conditions for the penalized Robin problem (P_α) (see Arada et al. [1]). Indeed, our numerical computations confirmed this issue. As an example, we show in detail the case $T = 1.58$ and y_d defined in (3.6).

For our numerical experiments we selected a fixed grid with $n_x = n_t = 101$ and used a standard central difference approximation of the Laplace operator with an implicit Euler scheme for the time integration to solve the differential equations numerically. To solving the optimal control problems, we applied a primal-dual active set strategy. For large α , we preferred a gradient projection method. For simplicity, we take first $u_0 \equiv 0$ as initial iterate to run the optimization methods.

In the case $\alpha < 1$, Conclusion 4.7 implies that the problem (P_α) admits a unique optimal bang-bang control. This is confirmed by our numerical experience, even for $\alpha = 1$, cf. Fig. 9.

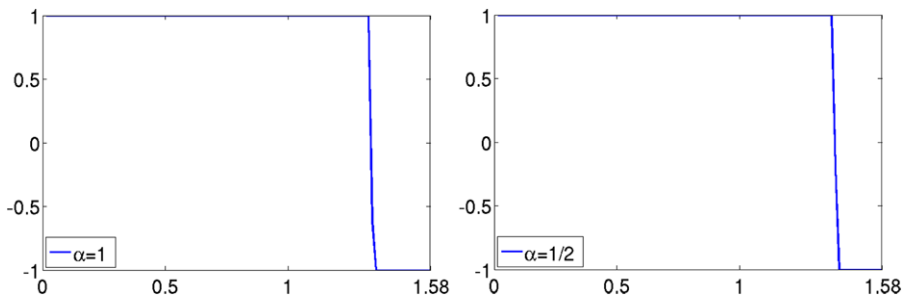


Fig. 9 Optimal control of (P_α) computed for $T = 1.58$, y_d defined in (3.6) and $\alpha = 1, \frac{1}{2}$

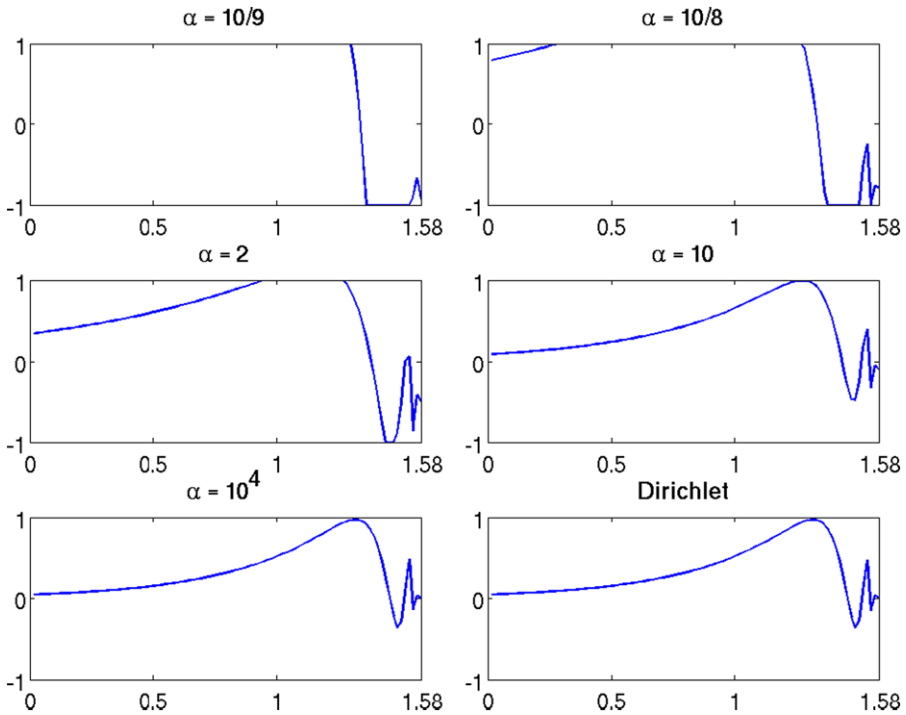


Fig. 10 Optimal control of (\mathcal{P}_D) and (\mathcal{P}_α) , for $\alpha = \frac{10}{9}, \frac{10}{8}, 2, 10$ and 10^4

Figure 10 shows the numerical solution of (\mathcal{P}_α) for $\alpha = \frac{10}{9}, \frac{10}{8}, 2, 10$ and 10^4 , as well as the numerical optimal control of the Dirichlet problem (\mathcal{P}_D) . One can easily see that for large α the solution of (\mathcal{P}_α) approaches the solution of (\mathcal{P}_D) . It is remarkable that for $\alpha > 1$ the optimal control is no longer bang-bang. Moreover, it holds $\ker S_T \neq \{0\} \forall T > 0$, which can be seen as follows: Let us take an arbitrary control $u \in L^\infty(0, \frac{T}{2}), u \neq 0$ and fix $y_d := S_{\frac{T}{2}}u$. By virtue of null-controllability, $0 \in R_{\frac{T}{2}}(y_d, L^\infty)$, there exists $v \in L^\infty(0, \frac{T}{2}), v \neq 0$, with $S_{\frac{T}{2}}v = 0$. Setting

$$\tilde{u}(t) = \begin{cases} u(t), & t \in [0, \frac{T}{2}), \\ v(t - \frac{T}{2}), & t \in [\frac{T}{2}, T], \end{cases}$$

we get $S\tilde{u} = 0$. Consequently, an optimal control \bar{u} of (\mathcal{P}_α) is not necessarily unique if \bar{u} belongs to the interior of U_{ad} , since $\bar{u} + \varepsilon u$ is also optimal for $u \in \ker S_T$ and $\varepsilon > 0$ such that $\bar{u} + \varepsilon u \in U_{ad}$. Indeed, we observed numerically that the optimal control \bar{u} of $(\mathcal{P}_\alpha), \alpha > 1$, depends on the initial iterate u_0 . The left frame of Fig. 12 shows the optimal controls of $(\mathcal{P}_\alpha), \alpha = 10$, obtained by starting with $u_0 \equiv 1, -1$ and 0, respectively.

To overcome these difficulties, we added a Tikhonov regularization term $\frac{\eta}{2} \|u\|_{L^2(0,T)}^2, \eta > 0$, to the functional J . This yields the coercivity of

$$\tilde{J}(u, y) := \frac{1}{2} \|y(\cdot, T) - y_d\|_{L^2(0,1)}^2 + \frac{\eta}{2} \|u\|_{L^2(0,T)}^2,$$

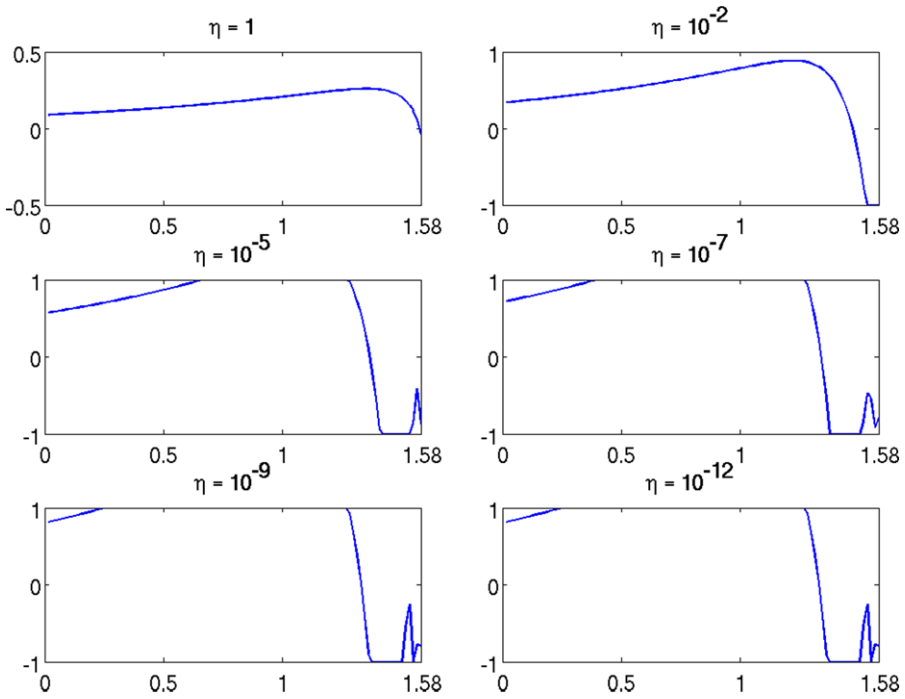


Fig. 11 Optimal control of (6.1) for $\alpha = \beta = \frac{10}{8}$ and $\eta = 1, 10^{-2}, 10^{-5}, 10^{-7}, 10^{-9}$ and 10^{-12}

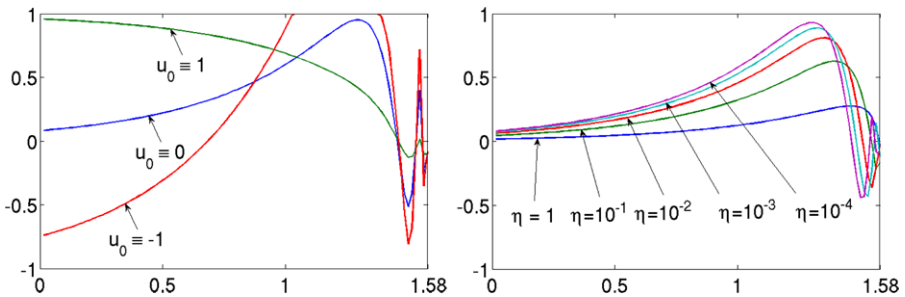


Fig. 12 Optimal controls for $\alpha = 10$, different initial iterates u_0 (left) and Tikhonov parameters η (right)

and consequently the uniqueness of the optimal control \bar{u}_η of the problem

$$\min \tilde{J}(u, y) \text{ subject to (1.1) and to (1.3).} \tag{6.1}$$

Another advantage of this regularization process is the stability of the generated results with respect to perturbations arising from numerical effects.

In [16, Chap. 1, Sect. 2] it is shown that $\|\bar{u}_\eta - \bar{u}_{min}\|_{L^2(0,T)} \rightarrow 0$ as $\eta \rightarrow 0$, where \bar{u}_{min} is the *minimum norm solution* of the optimal control problem,

$$\bar{u}_{min} = \min\{\|\tilde{u}\| \mid J(\tilde{u}, y(\tilde{u})) = \min J(u, y(u)), \tilde{u} \in L^2(0, T)\}.$$

Figure 11 shows the optimal control of the problem (6.1) when $\alpha = \beta = 10/8$ and $\eta \in \{1, 10^{-2}, 10^{-5}, 10^{-7}, 10^{-9}, 10^{-12}\}$. We did not estimate the precision of the ap-

proximation by computing the relative L^2 -error of \bar{u}_η . However, the numerical calculations showed that $\bar{u}_\eta \rightarrow \bar{u}$, as $\eta \rightarrow 0$, where \bar{u} is the optimal control of (\mathcal{P}_α) we got for the initial iterate $u_0 \equiv 0$ (cf. top right frame of Fig. 10). A similar situation is also illustrated in Fig. 12 for $\alpha = 10$, where \bar{u}_η tends to the solution of (\mathcal{P}_α) , as $\eta \rightarrow 0$, which was obtained for the same u_0 .

Appendix: Further estimates for the Robin problem

Here, we finish the discussion of Example 2, where we still have to exclude further zeros of $p(1, \cdot, \bar{\tau})$ on $(T_2, 1.5)$, $[1.5, 1.55]$ and $(1.55, 1.57]$.

Case $t \in (T_2, 1.5)$: As before, for $t \in (T_2, 1.5)$ we have

$$\sum_{n=4}^\infty C'_n(t)|D_n(\tau)| \leq \sum_{n=4}^\infty C'_n(1.5)|D_n(\tau)| \leq 2.26 \cdot 10^{-2} \cdot \sum_{n=3}^\infty q_{1.5}^n,$$

where $q_{1.5} = e^{-3\pi^2(1.58-1.5)} \in [0.0936, 0.09361]$, hence $\sum_{n=3}^\infty q_{1.5}^n = \frac{1}{1-q_{1.5}} - 1 - q_{1.5} - q_{1.5}^2 < 9.0501 \cdot 10^{-4}$ and

$$\sum_{n=4}^\infty C'_n(t)|D_n(\tau)| \leq 2.05 \cdot 10^{-5}.$$

Taking into account (3.21), we infer

$$\begin{aligned} \sum_{n=1}^3 C'_n(t)D_n(\tau_1) &\geq C'_1(1.5)D_1(\tau_1) + C'_2(T_2)D_2(\tau_1) + C'_3(1.5)D_3(\tau_1) \\ &> 0.5091777 \cdot (-6.573986 \cdot 10^{-4}) + 0.2613737 \cdot 0.01994057 \\ &\quad + 0.0693151 \cdot (-0.0240712) \\ &> 0.0032. \end{aligned}$$

Therefore $\frac{\partial}{\partial t} p(1, \cdot, \tau_1) > 0$ on $(T_2, 1.5)$, and with $p(1, T_2, \tau_1) > 0$ we conclude $p(1, t, \tau_1) \forall t \in [T_2, 1.5]$.

We cannot proceed this way neither on $(1.5, 1.55)$ nor on $(1.55, 1.57)$, since

$$C'_1(t_2)D_1(\tau_1) + C'_2(t_1)D_2(\tau_1) + C'_3(t_2)D_3(\tau_1) < 0,$$

when $(t_1, t_2) \in \{(1.5, 1.55), (1.55, 1.57)\}$. Thus, we follow the idea used in the case $t \in (1.57, T)$.

Case $t \in [1.5, 1.55]$: Here $q_{1.55} = e^{-3\pi^2(1.58-1.55)} \in [0.4113691, 0.4113692]$ and

$$\sum_{n=3}^\infty q_{1.55}^n = \frac{1}{1-q_{1.55}} - 1 - q_{1.55} - q_{1.55}^2 < 0.118264,$$

therefore

$$\sum_{n=4}^{\infty} C_n(t)|D_n(\tau_1)| \leq \sum_{n=4}^{\infty} C_n(1.55)|D_n(\tau_1)| \leq c_0 \cdot \sum_{n=3}^{\infty} q_{1.55}^n < 3.01 \cdot 10^{-5}.$$

On the other hand, from (3.21) we get

$$\begin{aligned} \sum_{n=1}^3 C_n(t)D_n(\tau_1) &\geq C_1(1.55)D_1(\tau_1) + C_2(1.5)D_2(\tau_1) + C_3(1.55)D_3(\tau_1) \\ &> 0.7138522 \cdot (-6.573986 \cdot 10^{-4}) + 0.05695014 \cdot 0.01994057 \\ &\quad + 0.0132817 \cdot (-0.0240712) \\ &> 3.466 \cdot 10^{-4}. \end{aligned}$$

Therefore $p(1, \cdot, \tau_1) > 0$ on $[1.5, 1.55]$.

Case $t \in (1.55, 1.57]$: As before, $q_{1.57} = e^{-3\pi^2(1.58-1.57)} \in [0.743721, 0.743722]$ and

$$\sum_{n=3}^{\infty} q_{1.57}^n = \frac{1}{1 - q_{1.57}} - 1 - q_{1.57} - q_{1.57}^2 < 0.118264,$$

therefore

$$\sum_{n=4}^{\infty} C_n(t)|D_n(\tau_1)| \leq \sum_{n=4}^{\infty} C_n(1.55)|D_n(\tau_1)| \leq c_0 \cdot \sum_{n=3}^{\infty} q_{1.55}^n < 4.084 \cdot 10^{-4}.$$

On the other hand, from (3.21) we get

$$\begin{aligned} \sum_{n=1}^3 C_n(t)D_n(\tau_1) &\geq C_1(1.57)D_1(\tau_1) + C_2(1.55)D_2(\tau_1) + C_3(1.57)D_3(\tau_1) \\ &> 0.7244983 \cdot (-6.573986 \cdot 10^{-4}) + 0.1024033 \cdot 0.01994057 \\ &\quad + 0.030422 \cdot (-0.0240712) \\ &> 8.334 \cdot 10^{-4}. \end{aligned}$$

Therefore $p(1, \cdot, \tau_1) > 0$ on $(1.55, 1.57]$.

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