Parabolic optimal control problems with combinatorial switching constraints Part II: Outer approximation algorithm*

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We consider optimal control problems for partial differential equations where the controls take binary values but vary over the time horizon, they can thus be seen as dynamic switches. The switching patterns may be subject to combinatorial constraints such as, e.g., an upper bound on the total number of switchings or a lower bound on the time between two switchings. In a companion paper [arXiv:2203.07121], we describe the L^p -closure of the convex hull of feasible switching patterns as intersection of convex sets derived from finite-dimensional projections. In this paper, the resulting outer description is used for the construction of an outer approximation algorithm in function space, whose iterates are proven to converge strongly in L^2 to the global minimizer of the convexified optimal control problem. The linear-quadratic subproblems arising in each iteration of the outer approximation algorithm are solved by means of a semi-smooth Newton method. A numerical example in two spatial dimensions illustrates the efficiency of the overall algorithm.

Keywords. PDE-constrained optimization, switching time optimization, outer approximation

1 Introduction

This paper is concerned with the design of an outer approximation algorithm for tailored convex relaxations of parabolic optimal control problems with combinatorial switching constraints, of the following form:

(P)
$$\begin{cases} \min \ J(y,u) = \frac{1}{2} \|y - y_{d}\|_{L^{2}(Q)}^{2} + \frac{\alpha}{2} \|u - \frac{1}{2}\|_{L^{2}(0,T;\mathbb{R}^{n})}^{2} \\ \text{s.t.} \ \partial_{t}y(t,x) - \Delta y(t,x) = \sum_{j=1}^{n} u_{j}(t) \psi_{j}(x) \quad \text{in } Q := \Omega \times (0,T), \\ y(t,x) = 0 \qquad \text{on } \Gamma := \partial \Omega \times (0,T), \\ y(0,x) = y_{0}(x) \qquad \text{in } \Omega, \\ \text{and} \quad u \in D. \end{cases}$$

Herein, T > 0 is a given final time and $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, is a bounded domain, i.e., a bounded, open, and connected set, with Lipschitz boundary $\partial\Omega$ in the sense of [22, Def. 1.2.2.1]. The form functions $\psi_i \in H^{-1}(\Omega)$, $j = 1, \ldots, n$, as well as the initial state $y_0 \in L^2(\Omega)$ are given.

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Moreover, $y_{d} \in L^{2}(Q)$ is a given desired state and $\alpha \geq 0$ is a Tikhonov parameter weighting the mean deviation from $\frac{1}{2}$. Finally,

$$D \subset \{ u \in BV(0,T; \mathbb{R}^n) : u(t) \in \{0,1\}^n \text{ f.a.a. } t \in (0,T) \}$$

denotes the set of feasible *switching controls*. The precise assumptions on D and examples for such a set are given in Section 2 below.

Problems of type (P) arise in various applications such as shifting of gear-switches in automotive engineering or valves in gas and water networks, see e.g., [19, 17, 32, 44, 24]. Thus, there exists a variety of different approaches for their numerical solution and we give a brief overview without claiming to be exhaustive. One approach is to discretize the optimal control problem, which typically leads to a large-scale mixed-integer nonlinear programming problem that is then solved by standard methods, see, e.g., [19, 33, 3, 18, 45]. Other methods employ convexifications accompanied by subsequent tailored rounding strategies. We exemplarily refer to [38, 39, 25, 29, 35, 34, 31, 41] and the references therein. If D imposes a bound on the BV-seminorm (as will also be the case in our setting), then the elements in Dare determined by a finite number of switching times. Several approaches rely on this observation and aim at optimizing these switching times, see e.g., [20, 14, 28, 15, 37, 36, 46]. In yet another class of methods, non-smooth penalty techniques, partly in combination with convexification, are used to account for the switching constraints in D. We refer to [10, 11, 12, 9, 49] and the references therein.

In our companion paper [5], we propose an entirely different approach for the solution of (P). This approach is based on a tailored convexification of (P), which is built by cutting planes derived from finite-dimensional projections. The numerical experiments in [5] demonstrate that our convexification generally provides better dual bounds than the naive relaxation, which is obtained by replacing the binarity constraints $u \in \{0,1\}^n$ by $u \in [0,1]^n$ in the definition of D. Even more, the prototypical example in [5, Counterexample 3.1] shows that the naive relaxation does not give the closure of the convex hull of D in any $L^p(0,T;\mathbb{R}^n)$ in general. In addition, the naive relaxation may not benefit from the particular problem structure, as the the investigation of the min-up/min-down polytope in [30] demonstrates. The reason is that the number of facets depends heavily on the discretization as shown by [40].

By contrast, our approach provably generates the closure of the convex hull in the limit. To be more precise, it is shown in [5] that $\overline{\operatorname{conv}(D)} = \bigcap_{k \in \mathbb{N}} V_k$, with the closure taken in $L^p(0,T;\mathbb{R}^n)$, see Theorem 2.2 below. Herein, the sets V_k correspond to sets in \mathbb{R}^{M_k} that, for prominent examples, can be shown to be polytopes for which the separation problem is tractable; see [5, Section 3.1 and 3.2]. In this paper, we will combine the separation algorithm for V_k with the passage to the limit $k \to \infty$ in order to obtain an *outer approximation algorithm* whose iterates converge strongly in $L^2(0,T;\mathbb{R}^n)$ to the global minimizer of (P) with D replaced by $\overline{\operatorname{conv}(D)}$. Outer approximation algorithms are well-established methods for the solution of mixed-integer nonlinear programs, see, e.g., the classical references [13, 16], and have also proven to work for combinatorial optimal control problems involving PDEs [7]. It is to be underlined that the sets V_k are designed by means of finite dimensional projections of the control variable only, without any discretization of the PDE in (P). Thus, by addressing the PDE in function space, we avoid the curse of dimensionality caused by the widely used first-discretize-then-optimize approach.

The plan of the paper reads as follows: In Section 2, we state the standing assumptions on D and recall the main results of our companion paper [5] that will be needed for the construction and the analysis of our outer approximation algorithm. Section 3 is devoted to the convergence analysis of the outer approximation algorithm for $k \to \infty$. In each iteration, a linear-quadatic optimal control problem subject to additional inequality constraints is solved. This is done by means of a semi-smooth Newton method in function space presented in Section 4. The performance of the overall algorithm is tested in Section 5 based on a finite element discretization of a prototypical optimal control problem. Finally, Section A is dedicated to an existence result for Lagrange multipliers required for the design of the semi-smooth Newton method.

2 Preliminaries

The main objective of this paper is to develop an efficient solution approach for the convexification of (\mathbf{P}) given by

(PC)
$$\begin{cases} \min f(u) := J(Su, u) \\ \text{s.t.} \quad u \in \overline{\text{conv} D}^{L^p(0, T; \mathbb{R}^n)}. \end{cases}$$

Hereby, $S: L^2(0,T;\mathbb{R}^n) \to W(0,T) := H^1(0,T;H^{-1}(\Omega)) \cap L^2(0,T;H^1_0(\Omega))$ denotes the solution operator associated with the PDE in (P), which admits for every control function $u \in D \subset L^{\infty}(0,T;\mathbb{R}^n)$ a unique weak solution; see, e.g., [48, Chapter 3]. Note that the objective function $f: L^2(0,T;\mathbb{R}^n) \to \mathbb{R}$ is weakly lower semi-continuous because the mappings $u \mapsto \|Su - y_d\|_{L^2(Q)}^2$ and $u \mapsto \|u - \frac{1}{2}\|_{L^2(0,T;\mathbb{R}^n)}^2$ are both convex and lower semi-continuous, thus weakly lower semi-continuous, and the solution operator S is affine and continuous, thus weakly continuous. The set

$$D \subset \left\{ u \in BV(0,T;\mathbb{R}^n) \colon u(t) \in \{0,1\}^n \text{ f.a.a. } t \in (0,T) \right\}$$

of feasible switching controls is supposed to satisfy the two following assumptions:

- (D1) D is a bounded set in $BV(0,T;\mathbb{R}^n)$,
- (D2) D is closed in $L^p(0,T;\mathbb{R}^n)$ for some fixed $p \in [1,\infty)$,

where $BV(0,T;\mathbb{R}^n)$ denotes the set of all vector-valued functions with bounded variation, i.e.,

$$BV(0,T;\mathbb{R}^n) := \{ u \in L^1(0,T;\mathbb{R}^n) : u_i \in BV(0,T) \text{ for } i = 1, \dots, n \}$$

equipped with the norm

$$||u||_{BV(0,T;\mathbb{R}^n)} := ||u||_{L^1(0,T;\mathbb{R}^n)} + \sum_{j=1}^n |u_j|_{BV(0,T)}.$$

For controls $u \in D$ the BV-seminorm $|u_j|_{BV(0,T)}$ agrees with the minimal number of switchings of any representative of u_j with values in $\{0, 1\}$. More details on the space of bounded variation functions can be found in [2, Chap. 10].

The set D covers a wide range of combinatorial switching constraints, for instance, in the case of an upper bound on the total number of switchings the set is given as

(2.1)
$$D_{\max} := \left\{ u \in BV(0,T;\mathbb{R}^n) : \ u(t) \in \{0,1\}^n \text{ f.a.a. } t \in (0,T), \\ |u_j|_{BV(0,T)} \le \sigma_{\max} \ \forall j = 1,\dots,n \right\},$$

where $\sigma_{\max} \in \mathbb{N}$ is a given number.

Under the assumptions (D1) and (D2) on the set D, the control problem (P) admits a global minimizer and the convex hull of the feasible switching patterns can be fully described by cutting planes lifted from finite-dimensional projections; see [5]. For the latter, the set D is projected, by means of

(2.2)
$$\Pi \colon BV(0,T;\mathbb{R}^n) \ni u \mapsto \left(\langle \Phi_i, u \rangle\right)_{i=1}^M \in \mathbb{R}^M ,$$

to the finite-dimensional space \mathbb{R}^M , where $\Phi_i \in L^p(0,T;\mathbb{R}^n)^*$, $i = 1, \ldots, M$, are linear and continuous functionals, e.g., local averaging operators of the form

(2.3)
$$\langle \Phi_{(j-1)N+i}, u \rangle := \frac{1}{\lambda(I_i)} \int_{I_i} u_j \, \mathrm{d}t$$

for j = 1, ..., n with suitably chosen subintervals $I_i \subset (0, T)$, i = 1, ..., N, and M := n N. Each projection Π then gives rise to a relaxation of the closed convex hull of the set D in $L^p(0, T; \mathbb{R}^n)$, which we will use to derive outer approximations by linear inequalities.

Lemma 2.1 ([5, Lemma 3.2]). For any Π as in (2.2), we have

$$\overline{\operatorname{conv}(D)}^{L^p(0,T;\mathbb{R}^n)} \subseteq \{ v \in L^p(0,T;\mathbb{R}^n) \colon \Pi(v) \in C_{D,\Pi} \}$$

where

$$C_{D,\Pi} := \operatorname{conv}\{\Pi(u) \colon u \in D\} \subset \mathbb{R}^M$$

Note that, based on the general assumptions (D1) and (D2), it is easy to see that the finite dimensional set $C_{D,\Pi}$ is closed in \mathbb{R}^M for any projection and consequently, the set $\{v \in L^p(0,T;\mathbb{R}^n): \Pi(v) \in C_{D,\Pi}\}$ is convex and closed in $L^p(0,T;\mathbb{R}^n)$.

In addition, projections Π_k , for increasing k, can be designed in such a way that an outer description of all finite-dimensional convex hulls C_{D,Π_k} also leads to an outer description of the convex hull of D in function space.

Theorem 2.2 ([5, Thm. 3.5]). For each $k \in \mathbb{N}$, let $I_1^k, \ldots, I_{N_k}^k$, $N_k \in \mathbb{N}$, be disjoint open intervals in (0,T) such that

- (i) $\bigcup_{i=1}^{N_k} \overline{I_i^k} = [0, T]$ for all $k \in \mathbb{N}$,
- (ii) $\max_{i=1,\dots,N_k} \lambda(I_i^k) \to 0 \text{ for } k \to \infty, \text{ and }$
- (iii) for each $r \in \{1, \ldots, N_{k+1}\}$ there exists $i \in \{1, \ldots, N_k\}$ such that $I_r^{k+1} \subseteq I_i^k$, i.e., the intervals form a nested sequence.

Set $M_k := n N_k$ and define projections $\Pi_k : BV(0,T;\mathbb{R}^n) \to \mathbb{R}^{M_k}$, for $k \in \mathbb{N}$, by

(2.4)
$$\langle \Phi_{(j-1)N_k+i}^k, u \rangle := \frac{1}{\lambda(I_i^k)} \int_{I_i^k} u_j(t) dt$$

for $j = 1, \ldots, n$ and $i = 1, \ldots, N_k$. Moreover, set

$$V_k := \{ v \in L^p(0,T;\mathbb{R}^n) \colon \Pi_k(v) \in C_{D,\Pi_k} \} .$$

Then $V_k \supseteq V_{k+1}$ for all $k \in \mathbb{N}$ and

(2.5)
$$\overline{\operatorname{conv}(D)}^{L^p(0,T;\mathbb{R}^n)} = \bigcap_{k \in \mathbb{N}} V_k .$$

Compared to Theorem 3.5 in [5], the assumption (iii) in the above theorem is additional. It is easy to see that it guarantees $V_k \supseteq V_{k+1}$ for all $k \in \mathbb{N}$, considering that each entry of Π_k is a convex combination of entries of Π_{k+1} . The second assertion (2.5) has been proven in [5].

3 Outer approximation algorithm

In the following, we explain how to address the convexified problem (PC) by an outer approximation approach. We use the outer descriptions of the sets $C_{D,\Pi}$ appearing in (2.5) to cut off any control $u \in L^p(0,T; \mathbb{R}^n)$ violating some of the conditions $\Pi(u) \in C_{D,\Pi}$.

More formally, we first fix an operator $\Pi: BV(0,T;\mathbb{R}^n) \ni u \mapsto (\langle \Phi_i, u \rangle)_{i=1}^M \in \mathbb{R}^M$ such that $\Pi(u) \notin C_{D,\Pi}$ holds. Since the convex set $C_{D,\Pi}$ is closed in \mathbb{R}^M , it is the intersection of its supporting half spaces and can be described by linear inequality constraints. The number of necessary half spaces can be infinite in general [5, Ex. 3.6], but for many practically relevant

constraints D, it turns out to be finite; see [5, Sect. 3.1 and 3.2]. Let us define the set of all valid linear inequalities for $C_{D,\Pi}$ as

$$H_{D,\Pi} = \{ (a,b) \in [-1,1]^M \times \mathbb{R} : a^\top w \le b \; \forall w \in C_{D,\Pi} \} ,$$

where $a \in [-1,1]^M$ can be assumed without loss of generality by scaling. To cut off the infeasible control u, we choose a violated linear inequality constraint and add this constraint to the problem. For the rest of this section, we assume that the local averaging operators satisfy the conditions (i)–(iii) of Theorem 2.2. Our outer approximation algorithm for (PC)then reads as follows:

Algorithm 1 Outer approximation algorithm for (PC)

1: Set $k = 0, T_0 = \emptyset, I_1^0 = (0, T)$ and $N_0 = 1$. 2: Solve $\begin{cases} \min \quad f(u) \\ \text{s.t.} \quad u \in [0,1]^n \quad \text{a.e. in } (0,T), \\ \quad a^\top \Pi(u) \le b \quad \forall (\Pi,a,b) \in T_k \ . \end{cases}$ (PC_k) Let u^k be the optimal solution. 3: if $u^k \in \overline{\operatorname{conv} D}^{L^p(0,T;\mathbb{R}^n)}$ then

return u^k as optimal solution. 4: 5: **else** Determine intervals I_i^{k+1} , $1 \le i \le N_{k+1}$, such that $\Pi_{k+1}(u^k) \notin C_{D,\Pi_{k+1}}$. Find an optimizer $(a_{k+1}, b_{k+1}) \in \arg\max_{(a,b)\in H_{D,\Pi_{k+1}}} (a^{\top}\Pi_{k+1}(u^k) - b)$. 6: 7: Set $T_{k+1} = T_k \cup \{(\Pi_{k+1}, a_{k+1}, b_{k+1})\}, k = k+1 \text{ and go to } 2.$ 8: 9: end if

Some remarks on Algorithm 1 are in order. First note that, by the standard direct method of calculus of variations, one can easily show the existence of a global minimizer for (PC_k) and its uniqueness if the Tikhonov parameter α is positive. Step 7 of the algorithm is well defined since $C_{D,\Pi_{k+1}} \neq \emptyset$ and hence b is bounded from below. Moreover, Step 6 is well defined due to (2.5). Consequently, an important subproblem in the outer approximation algorithm consists in determining appropriate intervals I_i of the local averaging operators, such that for a given u^k it holds $\Pi(u^k) \notin C_{D,\Pi}$. In view of Theorem 2.2, the desired property $\Pi(u^k) \notin C_{D,\Pi}$ follows as soon as Π is defined by a large enough number of small enough intervals, and remains valid for all further refinements. Note, however, that Step 6 does not exclude to set $\Pi_{k+1} = \Pi_k$ if this suffices to cut off u^k . Finally, we emphasize that the stopping criterion in Step 3 is rather symbolic; in general, it can be verified only by showing that no further violated cutting planes exist, for any projection.

From a practical point of view, we obtain u^k by solving the parabolic optimal control problem (PC_k), so that we know u^k only subject to a given discretization of (0,T); see Section 4 for more details on the numerical solution of (PC_k) . One could thus argue that the best possible approach is to choose the intervals I_i exactly as given by this discretization. This may be a feasible approach provided that the finite-dimensional separation algorithm for $C_{D,\Pi}$, needed in Step 7, is fast enough to deal with problems of large dimension M, as it is the case for a switch-wise upper bound on the total number of shiftings as defined in (2.1); see Section 5. However, one cannot expect such a fast separation algorithm for general switching constraints, so that it may be necessary to restrict oneself to a smaller number of intervals.

We now investigate the convergence behavior of Algorithm 1. It turns out that choosing the most violated inequality in Step 7 is crucial to guarantee convergence; this is a common choice in semi-infinite programming [23]. In addition, we have to require additional assumptions on the partitions of (0, T) used for the construction of the local averaging operators: besides the hypotheses (i)–(iii) from Theorem 2.2, we have to assume that the partitions are quasi-uniform. For this purpose, we introduce

$$\tau_k := \min_{1 \le i \le N_k} \lambda(I_i^k) \quad \text{and} \quad h_k := \max_{1 \le i \le N_k} \lambda(I_i^k),$$

and require

Assumption 3.1. There exists $\kappa > 0$ such that $h_k \leq \kappa \tau_k$ for every $k \in \mathbb{N}$.

Given this assumption, we can prove the following

Theorem 3.2. Assume that Algorithm 1 does not stop after a finite number of iterations and the sequence $I_1^k, \ldots, I_{N_k}^k$ resulting from Step 6 is constructed such that it meets the assumptions (i)–(iii) from Theorem 2.2 and Assumption 3.1. Suppose in addition that the Tikhonov parameter α is positive. Then the sequence $\{u^k\}_{k\in\mathbb{N}}$ converges strongly in $L^2(0,T;\mathbb{R}^n)$ to the unique global minimizer of (PC).

Proof. Thanks to the box constraint $u \in [0,1]^n$ a.e in (0,T), the sequence $\{u^k\}_{k\in\mathbb{N}}$ is bounded in $L^{\infty}(0,T;\mathbb{R}^n)$ so that there exists a weakly-* converging subsequence, denoted by $u^{k_m} \to^* u^*$ in $L^{\infty}(0,T;\mathbb{R}^n)$. Since weak-* convergence implies weak convergence in $L^p(0,T;\mathbb{R}^n)$ and the local averaging operators are clearly weakly continuous, we thus get $\Pi(u^{k_m}) \to \Pi(u^*)$ for $m \to \infty$ and any projection Π occurring in Algorithm 1. Additionally, the set

$$\{u \in L^p(0,T;\mathbb{R}^n) : u \in [0,1]^n \text{ a.e. in } (0,T)\}$$

is convex and closed, hence weakly closed, and therefore $u^{\star}(t) \in [0,1]^n$ a.e. in (0,T). Consequently, u^{\star} is feasible for all problems $(\mathbf{PC}_k), k \in \mathbb{N}$. The optimality of u^{k_m} for (\mathbf{PC}_{k_m}) now implies $f(u^{k_m}) \leq f(u^{\star})$ and the weak lower semi-continuity of f thus gives

(3.1)
$$f(u^{\star}) \leq \liminf_{m \to \infty} f(u^{k_m}) \leq \limsup_{m \to \infty} f(u^{k_m}) \leq f(u^{\star}),$$

i.e., $f(u^{k_m}) \to f(u^*)$. Since $u \mapsto ||Su - y_d||^2_{L^2(Q)}$ and $u \mapsto ||u - \frac{1}{2}||^2_{L^2(0,T;\mathbb{R}^n)}$ are both convex and lower semi-continuous, thus weakly lower semi-continuous, the convergence of the objective and the assumption $\alpha > 0$ imply

$$||u^{k_m} - \frac{1}{2}||^2_{L^2(0,T;\mathbb{R}^n)} \to ||u^{\star} - \frac{1}{2}||^2_{L^2(0,T;\mathbb{R}^n)}.$$

Since weak and norm convergence in Hilbert spaces imply strong convergence, this gives the strong convergence of $\{u^{k_m}\}_{m\in\mathbb{N}}$ to u^* in $L^2(0,T;\mathbb{R}^n)$.

We next prove

(3.2)
$$u^{\star} \in V_{\ell} = \{ v \in L^{p}(0,T;\mathbb{R}^{n}) \colon \Pi_{\ell}(v) \in C_{D,\Pi_{\ell}} \} \quad \forall \ell \in \mathbb{N}.$$

To this end, let $\ell \in \mathbb{N}$ be arbitrary, but fixed, and choose

$$(\bar{a}, \bar{b}) \in \operatorname{argmax}_{(a,b)\in H_{D,\Pi_{\ell}}}(a^{\top}\Pi_{\ell}(u^{\star}) - b).$$

Then we obtain for every $k \ge \ell$ and every $u \in L^p(0,T;\mathbb{R}^n)$ that

$$\bar{a}^{\top} \Pi_{\ell}(u) = \sum_{j=1}^{n} \sum_{i=1}^{N_{\ell}} \bar{a}_{(j-1)N_{\ell}+i} \frac{1}{\lambda(I_{i}^{\ell})} \int_{I_{i}^{\ell}} u_{j}(t) dt$$

$$= \sum_{j=1}^{n} \sum_{i=1}^{N_{\ell}} \bar{a}_{(j-1)N_{\ell}+i} \frac{1}{\lambda(I_{i}^{\ell})} \sum_{I_{r}^{k} \subseteq I_{i}^{\ell}} \int_{I_{r}^{k}} u_{j}(t) dt$$

$$= \sum_{j=1}^{n} \sum_{i=1}^{N_{\ell}} \sum_{I_{r}^{k} \subseteq I_{i}^{\ell}} \underbrace{\bar{a}_{(j-1)N_{\ell}+i} \frac{\lambda(I_{r}^{k})}{\lambda(I_{i}^{\ell})}}_{=:(\tilde{a}_{k})_{(j-1)N_{k}+r}} \frac{1}{\lambda(I_{r}^{k})} \int_{I_{r}^{k}} u_{j}(t) dt = \tilde{a}_{k}^{\top} \Pi_{k}(u) .$$

Note that the vector $\tilde{a}^k = ((\tilde{a}_k)_1, \ldots, (\tilde{a}_k)_{M_k}) \in \mathbb{R}^{M_k}$, $M_k = n N_k$, is well defined, since the intervals are nested by assumption (iii) in Theorem 2.2. Thus the convergence of u^{k_m} to u^* yields

(3.4)
$$\bar{a}^{\top} \Pi_{\ell}(u^{\star}) - \bar{b} = \lim_{m \to \infty} \bar{a}^{\top} \Pi_{\ell}(u^{k_{m}}) - \bar{b}$$
$$= \lim_{m \to \infty} \tilde{a}^{\top}_{k_{m}+1} \Pi_{k_{m}+1}(u^{k_{m}}) - \bar{b}$$
$$= \lim_{m \to \infty} \frac{h_{k_{m}+1}}{\tau_{\ell}} \left[\frac{\tau_{\ell}}{h_{k_{m}+1}} (\tilde{a}^{\top}_{k_{m}+1} \Pi_{k_{m}+1}(u^{k_{m}}) - \bar{b}) \right]$$

Moreover, for every $u \in D$ and every $k \geq \ell$, we deduce from (3.3) and $(\bar{a}, \bar{b}) \in H_{D,\Pi_{\ell}}$ that $\tilde{a}_{k}^{\top}\Pi_{k}(u) = \bar{a}^{\top}\Pi_{\ell}(u) \leq \bar{b}$, such that (\tilde{a}_{k}, \bar{b}) induces a valid inequality for $C_{D,\Pi_{k}}$. Hence, for k sufficiently large, $\frac{\tau_{\ell}}{h_{k}}(\tilde{a}_{k}, \bar{b})$ induces a valid inequality as well, where the coefficients satisfy

$$\frac{\tau_{\ell}}{h_k} \left| (\tilde{a}_k)_{(j-1)N_k+r} \right| = \frac{\tau_{\ell}}{\lambda(I_i^{\ell})} \frac{\lambda(I_r^k)}{h_k} \left| \bar{a}_{(j-1)N_{\ell}+i} \right| \le \left| \bar{a}_{(j-1)N_{\ell}+i} \right| \le 1$$

for all j = 1, ..., n and all $r = 1, ..., N_k$. Thus $\frac{\tau_{\ell}}{h_{k_m+1}}(\tilde{a}_{k_m+1}, \bar{b}) \in H_{D, \Pi_{k_m+1}}$, provided that m is sufficiently large, which in turn gives

$$\frac{\tau_{\ell}}{h_{k_m+1}} \left(\tilde{a}_{k_m+1}^{\top} \Pi_{k_m+1}(u^{k_m}) - \bar{b} \right) \le a_{k_m+1}^{\top} \Pi_{k_m+1}(u^{k_m}) - b_{k_m+1},$$

because the most violated cutting plane is chosen in Step 7 of Algorithm 1. Together with (3.4), the latter yields

(3.5)
$$\bar{a}^{\top} \Pi_{\ell}(u^{\star}) - \bar{b} \leq \frac{1}{\tau_{\ell}} \liminf_{m \to \infty} h_{k_m+1}(a_{k_m+1}^{\top} \Pi_{k_m+1}(u^{k_m}) - b_{k_m+1}).$$

Since u^* is feasible for all (PC_k) as seen above, we obtain for the right hand side

$$\begin{aligned} h_{k_m+1} \left(a_{k_m+1}^\top \Pi_{k_m+1} (u^{k_m}) - b_{k_m+1} \right) \\ &= h_{k_m+1} \left(a_{k_m+1}^\top \Pi_{k_m+1} (u^{\star}) - b_{k_m+1} \right) + h_{k_m+1} a_{k_m+1}^\top \Pi_{k_m+1} (u^{k_m} - u^{\star}) \\ &\leq h_{k_m+1} a_{k_m+1}^\top \Pi_{k_m+1} (u^{k_m} - u^{\star}) \end{aligned}$$

and, since $a_{k_m+1} \in [-1, 1]^{M_{k_m+1}}$, we can further estimate

$$(3.6) \qquad \begin{aligned} |h_{k_m+1} \, a_{k_m+1}^{\dagger} \Pi_{k_m+1} (u^{k_m} - u^{\star})| \\ &\leq h_{k_m+1} \sum_{j=1}^{n} \sum_{i=1}^{N_{k_m+1}} \frac{1}{\lambda (I_i^{k_m+1})} \int_{I_i^{k_m+1}} |u_j^{k_m} - u_j^{\star}| \, \mathrm{d}t \\ &\leq \frac{h_{k_m+1}}{\tau_{k_m+1}} \sum_{j=1}^{n} \sum_{i=1}^{N_{k_m+1}} \int_{I_i^{k_m+1}} |u_j^{k_m} - u_j^{\star}| \, \mathrm{d}t \\ &\leq \kappa \sum_{j=1}^{n} \|u_j^{k_m} - u_j^{\star}\|_{L^1(0,T)} \to 0, \quad \text{as } m \to \infty, \end{aligned}$$

where we used Assumption 3.1 and the strong convergence of u^{k_m} to u^* . From (3.5) we now obtain $\bar{a}^{\top} \Pi_{\ell}(u^*) - \bar{b} \leq 0$ and thus $a^{\top} \Pi_{\ell}(u^*) - b \leq 0$ for all $(a, b) \in H_{D,\Pi_{\ell}}$ due to the choice $(\bar{a}, \bar{b}) \in \arg \max_{(a,b) \in H_{D,\Pi_{\ell}}} (a^{\top} \Pi_{\ell}(u^*) - b)$. This gives $u^* \in V_{\ell}$, as claimed. Since $\ell \in \mathbb{N}$ was arbitrary, we finally arrive at

$$u^{\star} \in \bigcap_{\ell \in \mathbb{N}} V_{\ell} = \overline{\operatorname{conv} D}^{L^{p}(0,T;\mathbb{R}^{n})}$$

where the equality was shown in Theorem 2.2, i.e., u^* is feasible for (PC). To show optimality, consider any $u \in L^p(0,T;\mathbb{R}^n)$ feasible for (PC). Then u is also feasible for (PC) $_{k_m}$) for every $m \in \mathbb{N}$, and the optimality of u^{k_m} implies $f(u^{k_m}) \leq f(u)$. Due to $f(u^{k_m}) \to f(u^*)$ by (3.1), we thus have the optimality of u^* .

Now, since $\alpha > 0$ by assumption, (PC) is a strictly convex problem such that u^* is the unique global minimizer of (PC). A well-known argument by contradiction then shows the strong convergence of the whole sequence $\{u^k\}_{k \in \mathbb{N}}$.

Remark 3.3. An inspection of the above proof allows the following modification of the quasiuniformity condition in Assumption 3.1: since the subsequence $\{u^{k_m}\}_{m\in\mathbb{N}}$ is bounded in $L^{\infty}(0,T;\mathbb{R}^n)$, Lebesgue's dominated convergence theorem gives that u^{k_m} converges strongly to u^* in $L^q(0,T;\mathbb{R}^n)$ for every $q < \infty$. With an estimate analogous to (3.6) and Hölder's inequality, one then sees that the condition

(3.7)
$$\sum_{i=1}^{N_k} h_k^{q'} \lambda (I_i^k)^{1-q'} \le C < \infty \quad \text{for all } k \in \mathbb{N}$$

is sufficient for the convergence result in (3.6). Herein, q' is the conjugate exponent and can thus be chosen arbitrarily close to 1. It is easily seen that Assumption 3.1 implies (3.7). Nevertheless, we decided to require the stronger Assumption 3.1, since it is more elementary and certainly more relevant from a practical point of view.

4 Solution of OCP-relaxations

It remains to explain how we solve the optimal control problems (PC_k) appearing in the outer approximation algorithm numerically. We first set down the KKT-condition for (PC_k) . For this purpose, we introduce the linear and continuous (and thus Fréchet differentiable) operator

$$\Psi \colon L^2(0,T;\mathbb{R}^n) \to L^2(0,T;H^{-1}(\Omega)), \quad (\Psi u)(t) = \sum_{j=1}^n u_j(t)\psi_j$$

as well as the solution operator $\Sigma : L^2(0,T; H^{-1}(\Omega)) \to W(0,T)$ of the heat equation with homogeneous initial condition, i.e., given $w \in L^2(0,T; H^{-1}(\Omega)), y = \Sigma(w)$ solves

$$\partial_t y - \Delta y = w$$
 in $L^2(0, T; H^{-1}(\Omega)), \quad y(0) = 0$ in $L^2(\Omega).$

Moreover, we introduce the function $\zeta \in W(0,T)$ as solution of

$$\partial_t \zeta - \Delta \zeta = 0$$
 in $L^2(0, T; H^{-1}(\Omega)), \quad \zeta(0) = y_0$ in $L^2(\Omega).$

The solution mapping $S: u \mapsto y$ in Section 2 is then given by $S = \Sigma \circ \Psi + \zeta$. In the following, we will consider S, Σ , and Ψ with different domains and ranges. With a little abuse of notation, we will always use the same symbols.

With Σ and Ψ at hand, the reduced objective in (PC_k) reads

$$f(u) = \frac{1}{2} \left\| \Sigma \Psi u + \zeta - y_{\rm d} \right\|_{L^2(Q)}^2 + \frac{\alpha}{2} \left\| u - \frac{1}{2} \right\|_{L^2(0,T;\mathbb{R}^n)}^2$$

such that, by the chain rule, its Fréchet derivative at $u \in L^2(0,T;\mathbb{R}^n)$ is given by

(4.1)
$$f'(u) = \Psi^* \Sigma^* (\Sigma \Psi u + \zeta - y_d) + \alpha (u - \frac{1}{2}) \in L^2(0, T; \mathbb{R}^n),$$

where we identified $L^2(0,T;\mathbb{R}^n)$ with its dual using the Riesz representation theorem. By standard methods, see e.g., [48, Sect. 3.6], one shows that the adjoint $\pi = \Sigma^* g$, for given $g \in L^2(0,T;H^{-1}(\Omega)) \hookrightarrow W(0,T)^*$, is the solution of the backward-in-time problem

(4.2)
$$-\partial_t \pi - \Delta \pi = g \text{ in } L^2(0, T; H^{-1}(\Omega)), \quad \pi(T) = 0 \text{ in } L^2(\Omega)$$

and is therefore an element of W(0,T), i.e., $\Sigma^* : L^2(0,T; H^{-1}(\Omega)) \to W(0,T)$ is the solution operator of (4.2). Furthermore, the adjoint of Ψ is given by

$$\begin{split} \Psi^* : L^2(0,T; H^1_0(\Omega)) &\to L^2(0,T; \mathbb{R}^n), \\ (\Psi^* w)(t) &= \left(\langle \psi_j, w(t) \rangle_{H^{-1}(\Omega), H^1_0(\Omega)} \right)_{j=1}^n \quad \text{f.a.a. } t \in (0,T). \end{split}$$

Now we have everything at hand to apply the results of Appendix A to obtain the following KKT conditions:

Proposition 4.1. Denote the inequality constraints associated with the cutting planes in (PC_k) by $Gu \leq b$ with $G : L^p(0,T;\mathbb{R}^n) \to \mathbb{R}^k$ and $b \in \mathbb{R}^k$. Assume moreover that a function $\hat{u} \in L^{\infty}(0,T;\mathbb{R}^n)$ and a number $\delta > 0$ exist such that

(4.3) $\delta \leq \hat{u}_i(t) \leq 1 - \delta \quad \text{for all } i = 1, \dots, n \text{ and } f.a.a. \ t \in (0, T),$

 $(4.4) G\hat{u} \le b.$

Then a function $\bar{u} \in L^{\infty}(0,T;\mathbb{R}^n)$ with associated state $\bar{y} = S(\bar{u}) \in W(0,T)$ is optimal for (\mathbf{PC}_k) if and only if Lagrange multipliers $\lambda \in \mathbb{R}^k$ and $\mu_a, \mu_b \in L^2(0,T;\mathbb{R}^n)$ and an adjoint state $p \in W(0,T)$ exist such that the following optimality system is fulfilled:

(4.5)
$$-\partial_t p - \Delta p = \bar{y} - y_d \quad in \ L^2(0,T; H^{-1}(\Omega)), \quad p(T) = 0 \quad in \ L^2(\Omega),$$

(4.6)
$$\Psi^* p + \alpha \left(\bar{u} - \frac{1}{2} \right) + \mu_b - \mu_a + G^* \lambda = 0 \quad a.e. \ in \ (0,T),$$

(4.7)
$$\mu_a \ge 0, \qquad \mu_a \bar{u} = 0, \qquad \bar{u} \ge 0 \quad a.e. \text{ in } (0,T),$$

(4.8)
$$\mu_b \ge 0, \quad \mu_b(\bar{u}-1) = 0, \quad \bar{u} \le 1 \quad a.e. \text{ in } (0,T),$$

(4.9)
$$\lambda \ge 0, \quad \lambda^{\top} (G\bar{u} - b) = 0, \quad G\bar{u} \le b .$$

Proof. In view of (4.1) and (4.2), the necessity of (4.5)–(4.9) immediately follows from Theorem A.2. Due to the convexity of the optimal control problem (PC_k) , these conditions are also sufficient for (global) optimality.

It is easily verified that the Slater condition (4.3) and (4.4) is satisfied when the switches must additionally satisfy certain combinatorial conditions at any point in time [5, Sect. 3.1] or in the presence of linear constraints on the switching points [5, Sect. 3.2], e.g., with $u \equiv 1/2$. Consequently, in most of the practically relevant classes of constraints D the Slater conditions are fulfilled.

The pointwise resp. componentwise complementarity systems can equivalently be expressed by nonlinear complementarity functions such as, e.g., the max- or min-function, which leads to the following equivalent system to (4.6)-(4.9):

$$\begin{split} \Psi^* p + \alpha (\bar{u} - \frac{1}{2}) + G^* \lambda \\ &+ \min \left(-\Psi^* p - G^* \lambda + \frac{\alpha}{2}, 0 \right) \\ &+ \max \left(-\Psi^* p - G^* \lambda - \frac{\alpha}{2}, 0 \right) = 0 \quad \text{a.e. in } (0, T), \\ \rho \lambda + \max(0, G\bar{u} + \rho \lambda - b) = 0, \end{split}$$

where $\rho > 0$ can be chosen arbitrarily. Herein, we use the same symbol for the componentwise mapping $\mathbb{R}^k \ni v \mapsto (\max(v_i, 0))_{i=1}^k \in \mathbb{R}^k$ and the max-operator in function space. In view of $p = \Sigma^* (\Sigma \Psi \bar{u} + \zeta - y_d)$ the optimality system is thus equivalent to $F(\bar{u}, \lambda) = 0$ with $F: L^2(0, T; \mathbb{R}^n) \times \mathbb{R}^k \to L^2(0, T; \mathbb{R}^n) \times \mathbb{R}^k$ defined by

(4.10)

$$F_{1}(u,\lambda) := \Psi^{*}\Sigma^{*}(\Sigma\Psi u + \zeta - y_{d}) + \alpha(u - \frac{1}{2}) + G^{*}\lambda + \min\left(-\Psi^{*}\Sigma^{*}(\Sigma\Psi u + \zeta - y_{d}) - G^{*}\lambda + \frac{\alpha}{2}, 0\right) + \max\left(-\Psi^{*}\Sigma^{*}(\Sigma\Psi u + \zeta - y_{d}) - G^{*}\lambda - \frac{\alpha}{2}, 0\right)$$

and

(4.11)
$$F_2(u,\lambda) = -\rho\lambda + \max(0, Gu + \rho\lambda - b)$$

We now use the concept of semi-smoothness as developed in [8], see also the work of [26], to solve the above optimality system by means of a semi-smooth Newton method. For this purpose, we need the following

Assumption 4.2. In addition to our standing assumptions, there are exponents q > 2 and 0 < s < 2/q such that the form functions satisfy $\psi_j \in H_0^s(\Omega)^*$, j = 1, ..., n, and the linear functionals from (2.3) fulfill $\Phi_i \in L^{q'}(0, T, \mathbb{R}^n)^*$, i = 1, ..., M, where q' is the conjugate exponent, i.e., 1/q + 1/q' = 1.

Note that this mild additional regularity assumption on the functionals Φ_i is satisfied by the local averaging operators considered throughout this paper.

Lemma 4.3. Under Assumption 4.2, the function F given by (4.10) and (4.11) is Newton (or slant) differentiable.

Proof. The proof is standard, but for convenience of the reader, we sketch the arguments. The operator Π is linear and continuous with respect to u such that

$$L^2(0,T;\mathbb{R}^n) \times \mathbb{R}^k \ni (u,\lambda) \mapsto Gu + \rho\lambda - b \in \mathbb{R}^k$$

is continuously Fréchet differentiable. Exploiting the chain rule [27, Lemma 8.15] and the Newton differentiability of $\mathbb{R}^k \ni w \mapsto \max(0, w) \in \mathbb{R}^k$ [26, Lemma 3.1], we have that the second component F_2 is Newton differentiable.

Furthermore, according to [26, Prop. 4.1(ii)], the mapping $v \mapsto \max(0, v)$ is Newton differentiable from $L^s(0,T;\mathbb{R}^n)$ to $L^r(0,T;\mathbb{R}^n)$ for $1 \leq r < s \leq \infty$. We obtain the required norm gap with s = q and r = 2 by utilizing the smoothing properties of the PDE solution operators Σ and Σ^* , respectively. For all θ satisfying $0 < \theta - 1/2 < 1/q$, there holds

$$W(0,T) \hookrightarrow L^q(0,T; (H^{-1}(\Omega), H^1_0(\Omega))_{\theta,1}),$$

where $(H^{-1}(\Omega), H^1_0(\Omega))_{\theta,1}$ denotes the real interpolation space, see e.g., [1, Sect. 1]. For the latter, [47, Chap. 4.6.1] yields

$$(H^{-1}(\Omega), H^1_0(\Omega))_{\theta,1} \hookrightarrow [H^{-1}(\Omega), H^1_0(\Omega)]_{\theta} = H^{2\theta-1}_0(\Omega).$$

Consequently, if we now choose $\theta = 1/2(s+1)$ (which is feasible due to our assumptions on s), then Σ and $\Sigma^* \max L^2(0,T; H^{-1}(\Omega))$ linearly and continuously into $L^q(0,T; H_0^s(\Omega))$. According to Assumption 4.2, $\Psi \colon v \mapsto \sum_{j=1}^n v_j \psi_j$ maps $L^{q'}(0,T; \mathbb{R}^n)$ linearly and continuously to $L^{q'}(0,T; H_0^s(\Omega)^*)$. Thus, the Radon-Nikodým property of $H_0^s(\Omega)$ implies

$$\Psi^*: L^q(0,T; H^s_0(\Omega)) = \left(L^{q'}(0,T; H^s_0(\Omega)^*)\right)^* \to L^q(0,T; \mathbb{R}^n),$$

and therefore

$$L^{2}(0,T;\mathbb{R}^{n}) \ni u \mapsto \Psi^{*}\Sigma^{*}(\Sigma\Psi u) + \zeta - y_{d}) \in L^{q}(0,T;\mathbb{R}^{n})$$

is affine and continuous and hence continuously Fréchet differentiable. Moreover, if we identify $\Phi_i^{\ell} \in L^{q'}(0,T;\mathbb{R}^n)^*$, $i = 1, \ldots, M_{\ell}$, for a projection Π_{ℓ} occurring in (PC_k) with its Riesz representative, denoted by the same symbol, then its adjoint operator Π_{ℓ}^* is given by $\mathbb{R}^{M_{\ell}} \ni v \mapsto \sum_{i=1}^{M_{\ell}} v_i \Phi_i^{\ell} \in L^{q'}(0,T;\mathbb{R}^n)^*$, such that $G^*\lambda$ is given as

$$G^*\lambda = \sum_{\ell=1}^k \sum_{i=1}^{M_\ell} \lambda_\ell \, a_i^\ell \Phi_i^\ell \in L^{q'}(0,T;\mathbb{R}^n)^* \cong L^q(0,T;\mathbb{R}^n)$$

and

$$\mathbb{R}^k \ni \lambda \mapsto G^* \lambda \in L^q(0,T;\mathbb{R}^n)$$

is linear and continuous, too. Hence, owing to the Newton differentiability of max and the chain rule, F_1 is also Newton differentiable.

Now, as F is Newton differentiable, we choose

(4.12)
$$H_m(\delta u, \delta \lambda) := \begin{pmatrix} \chi_{\mathcal{I}_m} \Psi^* \Sigma^* \Sigma \Psi \delta u + \alpha \, \delta u + \chi_{\mathcal{I}_m} G^* \delta \lambda \\ -\rho \, \chi_{\mathcal{N}_m} \delta \lambda + \chi_{\mathcal{B}_m} G \delta u \end{pmatrix}$$

as a generalized derivative of F at a given iterate $z^m := (u^m, \lambda^m)$ with the active and inactive sets for the box constraints defined (up to sets of zero Lebesgue measure) by

$$\begin{aligned} \mathcal{A}_{m}^{+} &:= \left\{ (t,j) \in (0,T) \times \{1,\dots,n\} : -(\Psi^{*}p^{m})(t)_{j} - (G^{*}\lambda)(t)_{j} - \frac{\alpha}{2} > 0 \right\}, \\ \mathcal{A}_{m}^{-} &:= \left\{ (t,j) \in (0,T) \times \{1,\dots,n\} : -(\Psi^{*}p^{m})(t)_{j} - (G^{*}\lambda)(t)_{j} + \frac{\alpha}{2} < 0 \right\}, \\ \mathcal{I}_{m} &:= (0,T) \times \{1,\dots,n\} \setminus \{\mathcal{A}_{m}^{+} \cup \mathcal{A}_{m}^{-}\}, \end{aligned}$$

where $p^m := \Sigma^* (\Sigma \Psi u^m + \zeta - y_d)$, and the active and inactive cutting planes

$$\mathcal{B}_m := \{ i \in \{1, \dots, k\} : (Gu^m)_i + \rho \lambda_i^m > b_i \}, \\ \mathcal{N}_m := \{1, \dots, k\} \setminus \mathcal{B}_m.$$

Moreover, by $\chi_{\mathcal{I}_m}, \chi_{\mathcal{A}_m^{\pm}} : L^2(0,T;\mathbb{R}^n) \to L^2(0,T;\mathbb{R}^n)$ and $\chi_{\mathcal{N}_m}, \chi_{\mathcal{B}_m} : \mathbb{R}^k \to \mathbb{R}^k$, we denote the respective characteristic functions.

To compute the next iterate, we solve the following semi-smooth Newton equation

(4.13)
$$H_m(z^{m+1} - z^m) = -F(z^m).$$

For the sake of simplicity, we omit the index m at the inactive and active sets in the following. By definition of the active sets, the restriction of the first block in (4.13) to \mathcal{A}^+ and \mathcal{A}^- , respectively, yields

$$u^{m+1} = 1$$
 a.e. in \mathcal{A}^+ and $u^{m+1} = 0$ a.e. in \mathcal{A}^-

and the second block of (4.13) restricted to \mathcal{N} implies $\lambda_{|\mathcal{N}|}^{m+1} = 0$. Therefore, we can restrict the semi-smooth Newton equation (4.13) to the active components $\lambda_{|\mathcal{B}|}^{m+1}$ and the inactive part of the optimal control $u_{|\mathcal{I}|}^{m+1} \in L^2(\mathcal{I}; \mathbb{R}^n)$ only, which leads to

(4.14)
$$(\alpha I + \Psi^* \Sigma^* \Sigma \Psi \chi_{\mathcal{I}}^*) u_{|\mathcal{I}}^{m+1} + G^* \chi_{\mathcal{B}}^* \lambda_{|\mathcal{B}}^{m+1}$$
$$= \Psi^* \Sigma^* (y_{\mathrm{d}} - \Sigma \Psi \chi_{\mathcal{A}^+}^* u_{|\mathcal{A}^+}^{m+1} - \zeta) + \frac{\alpha}{2} \quad \text{a.e. in } \mathcal{I}$$

and

(4.15)
$$\left(G\chi_{\mathcal{I}}^* u_{|\mathcal{I}}^{m+1} \right)_{\mathcal{B}} = b_{\mathcal{B}} - \left(G\chi_{\mathcal{A}^+}^* u_{|\mathcal{A}^+}^{m+1} \right)_{\mathcal{B}}$$

Note that $\chi_{\mathcal{I}}^*$ and $\chi_{\mathcal{A}^+}^*$ are the extension-by-zero operators mapping from $L^2(\mathcal{I}; \mathbb{R}^n)$ and $L^2(\mathcal{A}^+; \mathbb{R}^n)$, respectively, to $L^2(0, T; \mathbb{R}^n)$, while $(Gu)_{\mathcal{B}}$ denotes the restriction to indices in \mathcal{B} . The semi-smooth Newton algorithm is now given as follows.

Algorithm 2 Semi-smooth Newton method for (PC_k)

1: Choose $(u^0, \lambda^0) \in L^2(0, T; \mathbb{R}^n) \times \mathbb{R}^k$, set $\mathcal{A}^+ = \mathcal{A}^- = \mathcal{B} = \emptyset$ and m = 0. 2: Update the active and inactive sets $\mathcal{I}_m, \mathcal{A}_m^+, \mathcal{A}_m^-, \mathcal{B}_m$ and \mathcal{N}_m . 3: if $\mathcal{A}_m^+ = \mathcal{A}^+ \land \mathcal{A}_m^- = \mathcal{A}^- \land \mathcal{B}_m = \mathcal{B} \land m > 0$ then 4: return (u^m, λ^m) . 5: else 6: Compute (u^{m+1}, λ^{m+1}) by solving the linear system (4.14) and (4.15). 7: Set $\mathcal{A}^+ = \mathcal{A}_m^+, \mathcal{A}^- = \mathcal{A}_m^-, \mathcal{B} = \mathcal{B}_m$ and m = m + 1, return to 2. 8: end if It is well known (see, e.g., [27, Chap. 8]) that the algorithm converges locally superlinearly if all generalized derivatives appearing in the iteration are continuously invertible and their inverses admit a common uniform bound. In our case however, it is very likely that Gbecomes rank deficient if the number k of cutting planes is large, such that the system (4.14)-(4.15) is no longer uniquely solvable. In our numerical experiments, however, a moderate number of cutting planes always sufficed and the semi-smooth Newton equation in Step 6 of the algorithm always admitted a unique solution for sufficiently large α . In the case that $\alpha > 0$ is small, one can only expect local superlinear convergence of the algorithm and no longer global convergence, this was also observed in our numerical experiments and a globalization would be needed for such instances.

After each iteration of the outer approximation algorithm presented in the previous section, one has to solve a parabolic control problem (PC_k) with an additional cutting plane by Algorithm 2. Due to this iterative structure, it is crucial to speed up the algorithm by reoptimization. More precisely, we exploit the solution of the prior outer approximation iteration to initialize the active and inactive sets in Algorithm 2.

The value of the Tikhonov parameter is crucial for the performance of numerical methods for the solution of optimal control problems, as already indicated above. This concerns discretization error estimates as well as convergence of optimization algorithms and conditioning of linear systems of equations arising in the latter. In case of (P) however, the choice of α has no impact on the set of minimizers, as $u \in \{0, 1\}^n$ a.e. in (0, T) and hence the Tikhonov term is constant. However, the convex relaxations of (P) considered in this paper as well their optimal values are influenced by α . Thus, in order to improve the performance of Algorithm 2, a large value of α is favorable, but we expect that the quality of the dual bounds in a branch-and-bound framework will become worse for larger values of α . A detailed investigation of this interplay is subject to future research.

5 Performance of the algorithm

We test the potential of our approach presented in the previous sections by an experimental study. For this, we concentrate on the case of a single switch with an upper bound σ_{\max} on the number of switchings, i.e., we consider

$$D := \{ u \in BV(0,T) \colon u(t) \in \{0,1\} \text{ f.a.a. } t \in (0,T), \ |u|_{BV(0,T)} \le \sigma_{\max} \}.$$

However, we assume that u is fixed to zero before the time horizon, so that we count it as a shift if u is 1 at the beginning. The most violated inequality for a $\Pi(u) \notin C_{D,\Pi}$, needed in Step 7 of Algorithm 1, can then be computed in time O(M) [6]. This is fast enough to allow choosing as intervals I_1, \ldots, I_M for the projection exactly the ones given by the discretization in time. In particular, we do not need to refine the intervals in the course of the outer approximation algorithm. For given $w \in C_{D,\Pi}$, we thus compute the most violated inequality of the form

$$\sum_{j=1}^{m} (-1)^{j+1} w_{i_j} \le \left\lfloor \frac{\sigma_{\max}}{2} \right\rfloor,$$

where $i_1, \ldots, i_m \in \{2, \ldots, M\}$ is an increasing sequence of indices with $m - \sigma_{\max}$ odd and $m > \sigma_{\max}$, by choosing $\{i_1, i_3, \ldots\}$ as the local maxima of w and $\{i_2, i_4, \ldots\}$ as the local minima of w (excluding 1).

The outer approximation algorithm devised in Section 3 is implemented in C++, using the DUNE-library [42] for the discretization of the PDE. The source code can be downloaded at https://github.com/agruetering/dune-MIOCP. The spatial discretization uses a standard Galerkin method with continuous and piecewise linear functionals. For the state y and the desired temperature y_d we also use continuous and piecewise linear functionals in time,

while the temporal discretization for the controls chooses piecewise constant functionals. The resulting linear, symmetric systems (4.14) and (4.15) in each semi-smooth Newton iteration are solved by the minimum residual solver MIN-RES [21] equipped with a suitable scalar product, induced by the temporal mass matrix, reflecting the norm of $L^2(0, T, \mathbb{R}^n)$ and the Euclidean scalar product in \mathbb{R}^k , and preconditioned with

$$P = \begin{pmatrix} \alpha I & 0\\ 0 & \frac{1}{\alpha} G G^{\star} \end{pmatrix} \; .$$

Hereby, we approximate the spatial integrals in the weak formulation of the state and adjoint equation, respectively, by applying a Gauss-Legrendre rule with order 3. The discrete systems, arising by the discretization of the state and adjoint equation, are solved by a sequential conjugate gradient solver preconditioned with AMG smoothed by SSOR.

We consider exemplary the square domain $\Omega = [0, 1]^2$, the end time T = 2 and the form function $\psi(x) = 1.5 - 2(x_1 - 0.5)^2 - 2(x_2 - 0.5)^2$. Moreover, in order to produce challenging instances, we generate a control $u_d: [0,T] \to [0,1]$ with a total variation $|u_d|_{BV(0,T)} \gg \sigma_{\max}$ and choose the desired state y_d in such a way that u_d is the optimal solution of our relaxation as long as no cutting planes are added. More specifically, we randomly choose $\sigma = 11$ jump points $0 < t_1 < t_2 < \cdots < t_{\sigma} < T$ on the time grid. Then, we choose $u_d: [0,T] \to [0,1]$ as cubic spline on $[t_{i-1}, t_i]$, for $1 \le i \le \sigma + 1$, where $t_0 := 0$ and $t_{\sigma+1} := T$, with $u_d(t_0) = 0$ and $u_d(t_{\sigma+1}) = 0.5$. The latter condition guarantees $p^*(T) = 0$ for the adjoint state

$$p^{\star}(t,x) = -\alpha c(u_{\rm d}(t) - \frac{1}{2})\sin(\pi x_1)\sin(\pi x_2),$$

where c is the inverse of the value $\int_{\Omega} \psi(x) \sin(\pi x_1) \sin(\pi x_2) dx$ and α is the Tikhonov parameter. By setting

$$y_{\rm d}(t,x) := S(u_{\rm d}) + \partial_t p^{\star}(t,x) + \Delta p^{\star}(t,x),$$

the optimal solution of our relaxation without cutting planes is given as $u^* = u_d$ and p^* represents the optimal adjoint state. In the generation of the instance, we compute $S(u_d)$ on a time grid with $N_t = 400$ time intervals, whereas the outer approximation is performed on a coarser grid.

In all experiments, we use a uniform spatial triangulation of Ω with 30×30 nodes, while experimenting with different temporal resolutions. The Tikhonov parameter was always set to $\alpha = 10^{-2}$. For the update of active cutting planes we chose $\rho = 10^{-5}$; see Section 4. The cutting plane algorithm stops as soon as the violation of the most violated cutting plane falls below 1% of the right hand side, the control is considered feasible for (PC) in this case. Note that the validity of the lower bound is not compromised by this.

All computations have been performed on a 64bit Linux system with an Intel Xeon E5-2640 CPU @ 2.5 GHz and 32 GB RAM.

We first illustrate the development of lower bounds over time; see Figure 1. Here, we used a typical instance with $\sigma_{\text{max}} = 2$ and a time grid with $N_t = 100$ intervals. Each cross corresponds to the lower bound (y-axis) obtained after adding another cutting plane, where the x-axis represents the time needed (in CPU hours) to obtain this bound. It can be seen that the bounds improve very quickly in the first cutting plane iterations and then continue to increase slowly. When using the lower bounds within a branch-and-bound scheme, this suggests to generate only few cutting planes before resorting to branching. For comparison, we also show the development of lower bounds in case no reoptimization is used; this is marked by circles. It can be observed that reoptimization significantly decreases running times.

The Tikhonov term has an impact on the performance of Algorithm 1, as well as on the quality of the bounds. The larger α is, the worse the bounds become, but the faster the convex relaxations can be solved. This can also be observed in Figure 2, where we solved the same instance of Figure 1, i.e., we used the same desired state y_d , with different Tikhonov



Figure 1: Temporal development of bounds.

parameters. The results show that choosing a small α is generally favorable, but for very small α there occurs a trade-off between the quality of the dual bounds and the convergence rate. Within a branch-and-bound framework, one needs to empirically investigate whether a good quality or a quick computation of the dual bounds for small α have a greater influence on the overall performance.



Figure 2: Temporal development of bounds for different α .

We next show the typical behavior of the optimal solutions of the relaxation when adding more and more cutting planes. For the example shown in Figure 3, we again have $N_t = 100$ and $\sigma_{\max} = 2$. Before adding the first cutting plane, the total variation is not bounded by any constraint; we have $|u^0|_{BV(0,T)} = 8.74$ then. Adding cutting planes quickly changes the shape of the optimal solutions u^i as well as their total variation, which however does not necessarily decrease monotonously. We emphasize that neither the shape of u^i nor its total variation is directly relevant for our approach, since we only aim at computing as tight lower bounds as possible.

Finally, we investigate the impact of the number of time intervals chosen for the discretization. Figure 4 demonstrates the temporal development of lower bounds for different numbers N_t and $\sigma_{\text{max}} = 2$. For a better comparison, we recalculate the resulting lower bounds



Figure 3: Development of optimal solutions.

(y-axis) with a finer temporal discretization, namely $N_t = 400$; note that this may lead to non-monotonous bounds. We observe that a coarser time grid quickly leads to better bounds, however, the accuracy of the lower bounds suffers enormously. In fact, the bounds obtained for a given discretization may not remain valid for a finer temporal grid.



Figure 4: Development of lower bounds for refined time grid.

In a branch-and-bound scheme, where larger parts of the switching structure will be fixed by the branching decisions, an adaptive discretization of the problem may be rewarding. Such an approach could be practicable within our outer approximation algorithm in function space, this is left as future work.

A Existence of Lagrange multipliers

This appendix shows the existence of Lagrange-multipliers for box constraints and finitely many linear inequality constraints, as appearing in the relaxation (PC_k) . A similar result under slightly less restrictive assumptions is shown in [50], but, for convenience of the reader we present a proof based on standard arguments in detail. For that, we consider problems of the form

(A.1)
$$\begin{cases} \min & f(u) \\ \text{s.t.} & u_a(\xi) \le u(\xi) \le u_b(\xi) \quad \text{f.a.a. } \xi \text{ in } \Lambda \\ & Gu \le b \end{cases}$$

where $\Lambda \subset \mathbb{R}^d$, $d \in \mathbb{N}$, is bounded and Lebesgue-measurable and $f : L^2(\Lambda) \to \mathbb{R}$ is continuously Fréchet differentiable. Moreover, $G : L^2(\Lambda) \to \mathbb{R}^m$, $m \in \mathbb{N}$ is linear and bounded and $b \in \mathbb{R}^m$ is given. Finally, $u_a, u_b \in L^{\infty}(\Lambda)$ satisfy

(A.2)
$$u_a(\xi) + \delta \le u_b(\xi)$$
 f.a.a. $\xi \in \Lambda$

with some $\delta > 0$.

Note that $L^{\infty}(\Lambda) \hookrightarrow L^2(\Lambda)$, since Λ is bounded. We will frequently regard G and f as mappings with domain $L^{\infty}(\Lambda)$ and, with a little abuse of notation, these maps are denoted by the same symbols. Clearly, they are also Fréchet differentiable as mappings with domain in $L^{\infty}(\Lambda)$.

In the following, let $\bar{u} \in L^{\infty}(\Lambda)$ be a locally optimal solution of (A.1). If we define the convex set $C := \{u \in L^{\infty}(\Lambda) : Gu \leq b\}$, then (A.1) is equivalent to

(A.1)
$$\iff \begin{cases} \min & f(u) \\ \text{s.t.} & u - u_a \in K, \quad u_b - u \in K, \quad u \in C \end{cases}$$

with $K := \{v \in L^{\infty}(\Lambda) : v \geq 0 \text{ a.e. in } \Lambda\}$. Note that K admits a non-empty interior as subset of $L^{\infty}(\Lambda)$. Furthermore, due to the linearity and continuity of the mapping G from $L^{\infty}(\Lambda) \hookrightarrow L^{2}(\Lambda)$ to \mathbb{R}^{m} , the set C is convex and closed.

In addition to (A.2), we suppose that the Slater condition is fulfilled, i.e., we assume that there is a function $\hat{u} \in L^{\infty}(\Lambda)$ such that

(A.3)
$$G\hat{u} \le b, \quad u_a(\xi) + \rho \le \hat{u}(\xi) \le u_b(\xi) - \rho$$

with $\rho > 0$. Since Slater's condition implies Robinson's constraint qualification, [4, Theorem 3.9] yields the existence of Lagrange multipliers $\mu_a, \mu_b \in L^{\infty}(\Lambda)^*$ such that

(A.4)
$$\langle f'(\bar{u}) + \mu_b - \mu_a, u - \bar{u} \rangle_{L^{\infty}(\Lambda)^*, L^{\infty}(\Lambda)} \ge 0 \quad \forall u \in C,$$

(A.5)
$$\mu_b \in K^+, \quad \langle \mu_b, \bar{u} - u_b \rangle_{L^{\infty}(\Lambda)^*, L^{\infty}(\Lambda)} = 0, \quad \bar{u} \le u_b \text{ a.e. in } \Lambda,$$

(A.6)
$$\mu_a \in K^+, \quad \langle \mu_a, u_a - \bar{u} \rangle_{L^{\infty}(\Lambda)^*, L^{\infty}(\Lambda)} = 0, \quad u_a \leq \bar{u} \text{ a.e. in } \Lambda,$$

where the dual cone is given by

$$K^+ := \{ \nu \in L^{\infty}(\Lambda)^* : \langle \nu, v \rangle_{L^{\infty}(\Lambda)^*, L^{\infty}(\Lambda)} \ge 0 \quad \forall v \in K \} .$$

In view of the definition of C, the gradient equation in (A.4) is equivalent to

(A.7)
$$\langle f'(\bar{u}) + \mu_b - \mu_a, s \rangle_{L^{\infty}(\Lambda)^*, L^{\infty}(\Lambda)} \ge 0 \quad \forall s \in G^{-1} \operatorname{cone}(\mathbb{R}^m_- - (G\bar{u} - b)),$$

where cone denotes the conic hull and $\mathbb{R}^m_- := \{v \in \mathbb{R}^m : v \leq 0\}$. The conic hull is given by

$$\operatorname{cone}(\mathbb{R}^m_- - (G\bar{u} - b)) = \operatorname{cone}\left(\{-e_1, \dots, -e_m, -G\bar{u} + b\}\right)$$

and, as the conic hull of finitely many points in \mathbb{R}^m , it is therefore closed. For its polar cone we find by elementary calculus that

(A.8)
$$\operatorname{cone}(\mathbb{R}^m_- (G\bar{u} - b))^\circ = \operatorname{cone}\left(\{e_i : i \in \mathcal{A}\}\right),$$

where $\mathcal{A} := \{i \in \{1, ..., m\} : (Gu)_i = b_i\}$ and $e_i \in \mathbb{R}^m$, i = 1, ..., m, denote the Euclidean unit vectors. Moreover, the following holds true:

Lemma A.1. The set $G^* \operatorname{cone}(\mathbb{R}^m_- - (G\overline{u} - b))^\circ$ is a weakly-* closed subset of $L^\infty(\Lambda)^*$.

Proof. Because G maps $L^2(\Lambda)$ linearly and continuously to \mathbb{R}^m , there exist functionals $g_i \in L^2(\Lambda)^* \cong L^2(\Lambda), i = 1, ..., m$, such that

$$Gu = \left(\langle g_i, u \rangle \right)_{i=1}^m$$
.

With a slight abuse of notation, we denote the application of g_i to functions in $L^{\infty}(\Lambda)$ by the same symbol. Direct computation shows that

(A.9)
$$G^* : \mathbb{R}^m \to L^\infty(\Lambda)^*, \quad G^*\lambda = \sum_{i=1}^m \lambda_i g_i$$

such that (A.8) implies $G^* \operatorname{cone}(\mathbb{R}^m_- (G\bar{u} - b))^\circ = \operatorname{cone}(\{g_i : i \in \mathcal{A}\})$. By [4, Prop. 2.41], the set cone $(\{g_i : i \in \mathcal{A}\})$ is weak-* closed, so that the assertion follows.

Thanks to Lemma A.1, all prerequisites of the generalized Farkas lemma are fulfilled, see e.g., [43, Prop. 2.4.2]. Therefore, (A.7) is equivalent to the existence of a multiplicator $\lambda \in \operatorname{cone}(\mathbb{R}^m_- - (G\bar{u} - b)) = \operatorname{cone}(\{e_i : i \in \mathcal{A}\}), \text{ cf. (A.8), such that})$

(A.10)
$$-f'(\bar{u}) - \mu_b + \mu_a - G^* \lambda = 0 \text{ in } L^{\infty}(\Lambda)^*.$$

Now, we are in the position to prove the desired multiplier theorem:

Theorem A.2. Suppose that a Slater point fulfilling (A.3) exists and let \bar{u} be a locally optimal solution to (A.1). Then there exist Lagrange multipliers $\lambda \in \mathbb{R}^m$ and $\mu_a, \mu_b \in L^2(\Lambda)$ such that

(A.11) $f'(\bar{u}) + \mu_b - \mu_a + G^* \lambda = 0 \quad a.e. \text{ in } \Lambda,$

(A.12)
$$\mu_a \ge 0, \quad \mu_a(\bar{u} - u_a) = 0, \quad \bar{u} \ge u_a \quad a.e. \text{ in } \Lambda,$$

(A.13)
$$\mu_b \ge 0, \quad \mu_b(\bar{u} - u_b) = 0, \quad \bar{u} \le u_b \quad a.e. \text{ in } \Lambda,$$

(A.14)
$$\lambda \ge 0, \quad \lambda^{\top} (G\bar{u} - b) = 0, \quad G\bar{u} \le b .$$

Proof. Let $u \in L^{\infty}(\Lambda)$ with $u_a \leq u \leq u_b$ a.e. in Λ be arbitrary. Inserting $v = u - \bar{u}$ in (A.10), we obtain

$$0 = \langle f'(\bar{u}) + G^* \lambda, u - \bar{u} \rangle + \langle \mu_b, u - u_b \rangle + \langle \mu_b, u_b - \bar{u} \rangle + \langle \mu_a, u_a - u \rangle + \langle \mu_a, \bar{u} - u_a \rangle$$

$$\leq \langle f'(\bar{u}) + G^* \lambda, u - \bar{u} \rangle ,$$

where we used (A.5) and (A.6) for the last estimate. Since $f'(\bar{u}) \in L^2(\Lambda)^* \cong L^2(\Lambda)$ and G^* maps \mathbb{R}^m to $L^2(\Lambda)$ by the regularity of g_i , i = 1, ..., m, the last inequality is equivalent to

(A.15)
$$\int_{\Omega} (f'(\bar{u}) + G^* \lambda) (u - \bar{u}) \, \mathrm{d}\xi \ge 0 \quad \forall \, u \in L^{\infty}(\Lambda) : u_a \le u \le u_b \text{ a.e. in } \Lambda.$$

Now, we introduce the functions $\mu_a, \mu_b \in L^2(\Lambda)$ by

$$\mu_a(\xi) := \max\{(f'(\bar{u}) + G^*\lambda)(\xi), 0\}, \quad \mu_b(\xi) := -\min\{(f'(\bar{u}) + G^*\lambda)(\xi), 0\} \quad \text{a.e. in } \Lambda$$

and denote them by μ_a and μ_b , too, with a little abuse of notation. Then, by means of standard arguments as e.g., in [48, Thm. 2.29], one deduces (A.11), (A.12), and (A.13) from (A.15). Finally, (A.14) follows from $\lambda \in \text{cone}(\{e_i : i \in \mathcal{A}\})$ and $(Gu - b)_i = 0$ for all $i \in \mathcal{A}$.

Remark A.3. Theorem A.2 readily carries over to vector valued box constraints in \mathbb{R}^n as in (\mathbf{PC}_k) , but in order to keep the discussion concise, we restricted it to the scalar case here.

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