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Branch-and-Lift Algorithm for Deterministic Global Optimization in Nonlinear Optimal Control

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Abstract This paper presents a branch-and-lift algorithm for solving optimal control problems with smooth nonlinear dynamics and potentially nonconvex objective and constraint functionals to guaranteed global optimality. This algorithm features a direct sequential method and builds upon a generic, spatial branch-and-bound algorithm. A new operation, called lifting, is introduced, which refines the control parameterization via a Gram–Schmidt orthogonalization process, while simultaneously eliminating control subregions that are either infeasible or that provably cannot contain any global optima. Conditions are given under which the image of the control parameterization error in the state space contracts exponentially as the parameterization order is increased, thereby making the lifting operation efficient. A computational technique based on ellipsoidal calculus is also developed that satisfies these conditions. The practical applicability of branch-and-lift is illustrated in a numerical example.

Keywords Optimal control · Deterministic global optimization · Spatial branch-and-bound

1 Introduction

Finding globally optimal solutions to nonlinear optimal control problems is a practically relevant, yet challenging task. Although nonlinear optimal control methods and tools based on local optimization are satisfactory for many practical purposes, they can get trapped into local optima, possibly suboptimal by a large margin. For example, in controlling a car or a robot in the presence of obstacles, a local solver

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typically fails to determine whether passing a given obstacle on the right or left is optimal. Similar situations can occur in the field of control of (bio)chemical processes, as these processes can present complex and highly nonlinear behavior leading for instance to steady-state multiplicity. For such problems, it is often unclear how to initialize a local solver in order to find a control input leading to the best possible performance. Moreover, there are important classes of problems for which obtaining a certificate of global optimality is paramount. In the field of robust and scenario-integrated optimization for instance, a global solution of the lower-level program is required to check the feasibility of an upper-level point; see, e.g., [1].

Local optimization theory for optimal control problems is well developed, and there is a wide variety of local optimization algorithms for such problems [2–4]. As far as global optimization is concerned, only a few numerical approaches exist, however. The focus of this paper is on deterministic global optimization methods, and therefore we do not elaborate further on stochastic global optimal control algorithms, referring the reader to [5–7] for an overview. Concerning deterministic global optimal control algorithms, we distinguish two classes of algorithms next, namely indirect and direct methods.

Indirect Optimal Control Methods Have in common that they first analyze an optimal control problem in terms of its optimality conditions, prior to applying a numerical discretization. Two of the most important classes of indirect methods are:

1. The *Hamilton–Jacobi–Bellman (HJB) equation* approach, which leads to a global optimal control algorithm known under the name dynamic programming. This technique is based on Bellman's optimality principle, named after the work by Bellman in the late 1950s [8]. In practice, dynamic programming involves back-propagating the so-called optimal value function in the state space, which limits application to optimal control problems having no more than a few state variables. Nevertheless, the dynamic programming approach is advantageous in that it can deal with time-varying controls directly, and, most importantly, it can determine globally optimal solutions. For an overview of state-of-the-art global optimal control based on dynamic programming, we refer the reader to [9–11]. Note also that some optimal control problems, for instance problems with coupled boundary conditions, cannot be addressed easily within this approach.
2. The *Pontryagin Maximum Principle (PMP)*, which leads to a boundary-value problem that is amenable to numerical solution [2, 12, 13]. This approach relies on variational analysis in order to derive first-order necessary conditions for optimality [14]. However, the PMP only provides local optimality conditions, and, to the authors' best knowledge, no global optimal control algorithm has been developed based on this technique to date. Although it should be possible, at least in principle, to use the PMP to single out a set of candidate optimal controls, perhaps the major difficulty with this approach would be of combinatorial nature since the sequence and types of arcs in an optimal solution are not known a priori.

Direct Optimal Control Methods Approximate the optimal control problem by a finite-dimensional nonlinear programming (NLP) problem, which is then solved using standard numerical optimization algorithms. Three main variants of this approach are single shooting, multiple shooting, and orthogonal collocation.

1. The idea behind the *single shooting* approach, also known as the *direct sequential* method, is to parameterize the control trajectories. The response of the dynamic systems is regarded as a function of the control parameterization coefficients, which are the decision variables in a finite-dimensional NLP problem. The evaluation of the objective and constraint functions in the discretized NLP is via the numerical integration of the differential equations. This approach was originally introduced in a local optimization context [4, 15, 16], but it has more recently been extended to global optimization, see, for example, [17–23]. Note that all of these approaches have in common that they rely on branch-and-bound search [24] to solve the resulting NLP problem to guaranteed global optimality. Their practical applicability is currently limited to optimal control problems with a small number of decision variables only, up to about 10 variables. This is attributed to the fact that a fine control parameterization leads to an NLP problem with a large number of degrees of freedom and also that state-of-the-art enclosure methods for nonlinear parametric differential equations can result in rather conservative bounds or convex relaxations due to the wrapping effect. We note that such enclosure methods can scale poorly with the number of state variables as well, especially if no particular structure can be exploited in the equations.
2. The *multiple shooting* approach differs from single shooting in that the time horizon is first divided into a number of subintervals [25]. The state variables at the initial time of each subinterval become additional decision variables in the NLP problem, state continuity at the transition times is enforced by imposing extra constraints, and the rest of the approach remains analogous to single shooting. The multiple shooting approach is available in state-of-the-art optimal control software based on local optimization solvers [26, 27], where the block structure of the NLP problem is exploited within the underlying linear algebra routines for efficiency. This approach has not been used in a global optimization context to date, presumably due to the fact that larger NLP problems are usually more difficult to solve using branch-and-bound search.
3. In the *orthogonal collocation* approach, both the control and the state trajectories are parameterized, and the residuals of the differential equations are enforced as constraints at specified collocation times [28, 29]. In the context of local optimization, this approach is frequently used in combination with large-scale NLP solvers that exploit the block structure of the discretized optimization problem efficiently [3]. Concerning global optimization, the collocation approach presents the advantage that all of the objective and constraint functions become factorable, so that in principle standard global optimization solvers such as BARON [30, 31] can be applied directly. The attendant drawback of this approach, however, is the large number of variables and constraints, which often leads to prohibitive computational times as discussed in [32].

Summarizing the previous considerations, existing global optimal control algorithms based on dynamic programming have run-times that scale exponentially with the number of differential states. Global optimization algorithms based on direct methods, on the other hand, present worst-case run-times that scale exponentially with the number of optimization variables in the discretized NLP problem approximating the solution of the original optimal control problem. Moreover, a priori parameterization of the control functions in direct methods does not allow control over the accuracy of a given parameterization, and therefore this approach is not suitable for rigorous search of globally optimal solutions in optimal control problems.

This paper develops a new algorithm, named *branch-and-lift*, in order to mitigate these limitations. This algorithm features a direct sequential approach and involves refining the control parameterization during the search as a means to control the error introduced by the control parameterization. Similar to the work by Galperin and Zheng [33], the parameterization refinement process is based on Gram–Schmidt orthogonalization. We extend Galperin and Zheng's idea in two ways here:

(i) the spatial branch-and-bound algorithm is equipped with a new lifting step that enables systematic branching in an infinite-dimensional space, namely the space of bounded Lebesgue-integrable control functions; and,
(ii) conditions are given under which the image of the control parameterization error in the state space contracts exponentially as the parameterization order is increased, thereby making the lifting operation efficient (see Theorem 4.1).

Put together, these contributions lead to a global optimization algorithm for optimal control problems that is rigorous in the sense that it brackets the solution value of the optimal control problem. Moreover, finite convergence to an ϵ-suboptimal solution is established for certain classes of optimal control problems (see Theorem 5.1 and Corollaries 5.1 and 5.2). With regard to the contribution (ii), it is worth mentioning the convex relaxation technique for optimal control problems developed by [34], which could also be used to compute valid lower bounds in the proposed branch-and-lift algorithm. Concerning the contribution (i), mention should be made of the so-called "Russian Doll Algorithm" (RDA) proposed by [35] as a variant of branch-and-bound for constraint satisfaction problems. In RDA, the optimization is performed sequentially over subsets of increasing dimensions, thus presenting some similarities with the lifting operation in the branch-and-lift algorithm.

The remainder of this paper is organized as follows. A mathematical problem statement is given in Sect. 2. In Sect. 3 we review existing control parameterization strategies as well as branch-and-bound search applied to direct optimal control methods. In Sect. 4 we define the image of the control discretization error in state space and discuss its properties. The first main contribution of the paper is presented in Theorem 4.1, where exponential convergence of the image of the control discretization error is established under mild conditions. The proof is reported in Appendix A, and a computational technique based on ellipsoidal calculus that satisfies these conditions is discussed in Appendix B. The second principal contribution follows in Sect. 5, where the new lifting operation is introduced as a means to refine the control parameterization during the search, and where the branch-and-lift algorithm is described. The convergence properties of the branch-and-lift algorithm are also analyzed. We illustrate the practical applicability of branch-and-lift in Sect. 6 through a detailed numerical case study, before concluding the paper in Sect. 7.

2 Problem Statement

We consider nonlinear optimal control problems (OCPs) of the form

$$\mathcal{V} := \min_{x,u} \Psi\big(x(T)\big) \quad \text{s.t.} \quad \begin{cases} \dot{x}(t) = f(x(t)) + G(x(t))u(t), \\ x(0) = x_0, \\ x(t) \in \mathbb{F}_x(t), \\ u(t) \in \mathbb{F}_u(t), \end{cases} \tag{1}$$

where the constraints have to be satisfied for all t in a given time horizon $[0, T]$. Here, $x : [0, T] \to \mathbb{R}^{n_x}$ denotes the state vector with given initial value vector $x_0 \in \mathbb{R}^{n_x}$, and $u : [0, T] \to \mathbb{R}^{n_u}$ is a Lebesgue-integrable control input vector. Moreover, we introduce the following technical blanket assumptions:

A1: The Mayer term $\Psi : \mathbb{R}^{n_x} \to \mathbb{R}$ is a Lipschitz-continuous function.
A2: The functions $f : \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ and $G : \mathbb{R}^{n_x} \to \mathbb{R}^{n_x \times n_u}$ are smooth and globally Lipschitz-continuous.
A3: The constraint sets $\mathbb{F}_x(t) \subseteq \mathbb{R}^{n_x}$ are closed in $\mathbb{R}^{n_x}$ for all $t \in [0, T]$.
A4: The constraint sets $\mathbb{F}_u(t) \subset \mathbb{R}^{n_u}$ are compact in $\mathbb{R}^{n_u}$ for all $t \in [0, T]$.

The problem formulation (1) and the blanket Assumptions A1–A4 are introduced in an objective to keep the notation and analysis in the paper as simple as possible, although the methods presented in the following sections can be generalized to a wider class of problems. This includes OCPs having additional finite-dimensional parameters or the initial value as additional optimization variables; OCPs with periodic or more generally coupled boundary conditions and with mixed control-state path constraints; OCPs with nonautonomous right-hand side functions f and G; and OCPs having an additional Lagrange term in the objective function.

Assumption A2 that f and G are globally Lipschitz continuous is introduced so as to guarantee the existence and uniqueness of the differential equation solutions, thereby ruling out the possibility of a finite escape time. A discussion about how to extend the developed algorithms to the case that f and G are locally, yet not globally, Lipschitz continuous is provided at the end of Sect. 5. Moreover, the sets $\mathbb{F}_x(t)$ in Assumption A3 are assumed to be closed, but not necessarily compact. In particular, this includes the case that no state constraints are present in the problem.

The problem formulation (1) assumes that the control function u enters the right-hand side function affinely. While the reasons for making this assumption will be explained later, it is worth mentioning at this point that many controlled physical systems are naturally affine in their control variables. In mechanical systems, for instance, typical control inputs are forces or torques that enter affinely in the dynamic system via Newton's law, even in the presence of nonlinear centrifugal, friction, or Coriolis effects; in controlled chemical reactors too, feed rates normally enter the conservation equations affinely, despite the possible presence of nonlinear reaction or transfer terms; and similarly in electrical circuits, controlled potential differences enter charge conservation equations affinely, regardless of the presence of resistances, diodes, or other electric devices with nonlinear characteristics. Moreover, in the case that we encounter a nonlinear differential equation in u, a reformulation as (1) can be made under the additional assumption that u is Lipschitz continuous. This way, the original control u can be regarded as an extra state satisfying an auxiliary ODE of the form $\dot{u}(t) = v(t)$, where v is the new control variable subject to $-\mathcal{L} \leq v(t) \leq \mathcal{L}$, with $\mathcal{L}$ the Lipschitz constant of u on $[0, T]$.

2.1 Notation

Besides standard mathematical notation, we write $\mathbb{R}_+ := \{x \in \mathbb{R} \mid x \geq 0\}$ and $\mathbb{R}_{++} := \{x \in \mathbb{R} \mid x > 0\}$. Moreover, we denote by $\mathbb{S}^n_+ \subseteq \mathbb{R}^{n \times n}$ the set of all symmetric positive-semidefinite $(n \times n)$ matrices and by $\mathbb{S}^n_{++} \subseteq \mathbb{S}^n_+$ the set of symmetric positive-definite $(n \times n)$ matrices. We use

$$\mathcal{E}(c, Q) := \left\{ c + Q^{\frac{1}{2}} v \mid v \in \mathbb{R}^n, v^\mathsf{T} v \leq 1 \right\} \subseteq \mathbb{R}^n$$

to denote an ellipsoid with center $c \in \mathbb{R}^n$ and positive-semidefinite matrix $Q \in \mathbb{S}^n_+$, and we denote by

$$\mathbb{I}(c, r) := \left\{ v \in \mathbb{R}^n \mid -r \leq v - c \leq r \right\} \subseteq \mathbb{R}^n$$

the interval with midpoint $c \in \mathbb{R}^n$ and width $2r$, with $r \in \mathbb{R}^n_+$. Moreover, the function $\mathrm{mid}(\mathbb{I}(c, r)) = c$ returns the midpoint of an interval.

Given a compact set $X \subseteq \mathbb{R}^n$ and a norm $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$, we use the notation

$$\mathrm{diam}(X) := \max_{x, y \in X} \|x - y\|$$

for the associated diameter of the set X. Moreover, the power set of X, namely the set of subsets of X including the empty set, is denoted by $\mathcal{P}(X)$. The Minkowski sum and the Minkowski difference of two sets X and Y are defined, respectively, as

$$X \oplus Y := \{x + y \mid x \in X, y \in Y\} \quad \text{and} \quad X \ominus Y := \left\{ x \mid \{x\} \oplus Y \subseteq X \right\}.$$

Throughout the paper, all (time) trajectories are understood to be Lebesgue integrable, and all integrals are understood in the sense of Lebesgue; we denote by $L^2[0, T]^n$ the set of n-dimensional, L^2-integrable functions on the interval $[0, T]$. By an abuse of language, we say that a statement holds for all $t \in [0, T]$ at times, but mean that this statement holds for all $t \in [0, T] \setminus L_0$, where L_0 can be any subset of $[0, T]$ of zero Lebesgue measure.

By convention, the optimal value of a minimization (resp. maximization) problem is taken as $+\infty$ (resp. $-\infty$) if the constraints are infeasible; that is, $\mathcal{V} = \infty$ whenever problem (1) is infeasible.

3 Background

This section reviews and formalizes concepts for the direct sequential approach of optimal control and its application within spatial branch-and-bound. The formalism introduced in this section is used throughout the paper.

3.1 Control Parameterization

It has already been mentioned that direct methods parameterize the control trajectories, so that an optimal control problem is approximated by a finite-dimensional NLP. To formalize the concept of control parameterization, we start by introducing a sequence of L^2-integrable basis functions $\Phi_0, \Phi_1, \dots, \Phi_M : [0,T] \to \mathbb{R}$ that are orthogonal with respect to a given bounded weighting function $\mu : [0,T] \to \mathbb{R}_{++}$ and scaling factors $\sigma_0, \sigma_1, \dots, \sigma_M \in \mathbb{R}_{++}$:

$$\forall i, j \in \{0, \dots, M\}, \quad \frac{1}{\sigma_i} \int_0^T \Phi_i(\tau)\Phi_j(\tau)\mu(\tau)\,\mathrm{d}\tau = \delta_{i,j} := \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{otherwise.} \end{cases}$$

The Gram–Schmidt coefficients $a_0, \dots, a_M \in \mathbb{R}^{n_u}$ for an L^2-integrable function $\omega : [0,T] \to \mathbb{R}^n$ on the interval $[0,T]$ are defined as

$$\forall i \in \{0, \dots, M\}, \quad a_i := \frac{1}{\sigma_i} \int_0^T \omega(\tau)\Phi_i(\tau)\mu(\tau)\,\mathrm{d}\tau.$$

When it is clear from the context on which time interval the integral is evaluated, we make use of the following short-hand notation for the component-wise scalar product:

$$\forall \omega \in L^2[0,T]^n, \forall \zeta \in L^2[0,T], \quad \langle \omega, \zeta \rangle_\mu := \int_0^T \omega(\tau)\zeta(\tau)\mu(\tau)\,\mathrm{d}\tau.$$

The first $M+1$ Gram–Schmidt coefficients of a control input are ordered into the vector a of dimension $n_a = (M+1)n_u < \infty$ as follows:

$$a := \left(a_0^\mathsf{T}, \dots, a_M^\mathsf{T}\right)^\mathsf{T} \in \mathbb{R}^{n_a} \quad \text{with } a_i = \frac{1}{\sigma_i}\langle u, \Phi_i \rangle_\mu. \tag{2}$$

Fundamental properties of orthogonal decompositions of L_2-integrable functions are recalled in the next proposition.

Proposition 3.1 *Let u be L^2-integrable on $[0,T]$, and let the vector a be defined as in (2). The following statements hold:*

1. *The first $M+1$ Gram–Schmidt coefficients of the control parameterization defect term $(u - \sum_{i=0}^M a_i \Phi_i)$ are all equal to zero:*

$$\forall i \in \{0, \dots, M\}, \quad \left\langle u - \sum_{j=0}^M a_j \Phi_j, \Phi_i \right\rangle_\mu = 0.$$

2. *Bessel's inequality for the coefficient sequence $a_0, a_1, \dots, a_M$ is satisfied:*

$$\forall j \in \{1, \dots, n_u\}, \quad \sum_{i=0}^M \sigma_i (a_i)_j^2 \le \langle u_j, u_j \rangle_\mu.$$

Example 3.1 A piecewise constant control parameterization over $M+1$ stages of equal duration $h := \frac{T}{M+1}$ can be obtained by using the orthogonal functions

$$\forall i \in \{0, \dots, M\}, \quad \Phi_i(t) = \begin{cases} 1 & \text{if } ih \le t \le (i+1)h, \\ 0 & \text{otherwise,} \end{cases}$$

together with the weighting function $\mu(t) = 1$ and scaling factors $\sigma_i = h$ for all indices $i \in \{0, \dots, M\}$.

The direct single-shooting algorithm presented in the following section relies on control parameterization using orthogonal basis functions.

3.2 Direct Single Shooting Revisited

The main idea behind single-shooting algorithms is to approximate the infinite-dimensional optimal control problem (1) with a finite-dimensional NLP problem in the variables a, as defined previously in Sect. 3.1. In order to formalize this concept, we denote by $y(t,a)$ the solution of the parametric differential equation

$$\forall t \in [0,T], \quad \dot{y}(t,a) = f\big(y(t,a)\big) + G\big(y(t,a)\big)\left(\sum_{i=0}^{M} a_i \Phi_i(t)\right), \quad \text{with} \tag{3}$$

$$y(0,a) = x_0.$$

Note that $y(t,a)$ is well defined if the blanket Assumption A2 is satisfied. For any closed domain $\mathbb{A} \subseteq \mathbb{R}^{n_a}$, we introduce the finite-dimensional optimization problem

$$\mathcal{V}_M(\mathbb{A}) := \min_{a \in \mathbb{A}} \Psi\big(y(T,a)\big) \quad \text{s.t.} \quad \begin{cases} y(t,a) \in \mathbb{F}_x(t), \\ \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t), \end{cases} \tag{4}$$

where the constraints have to be satisfied for all $t \in [0,T]$. The single-shooting approach computes the optimal value $\mathcal{V}_M(\mathbb{R}^{n_a})$, and this value yields an upper bound on the actual optimal value $\mathcal{V}$ of the optimal control problem (1):

$$\mathcal{V}_M\big(\mathbb{R}^{n_a}\big) \ge \mathcal{V}. \tag{5}$$

Moreover, because Problem (4) yields an optimization problem with a finite number of decision variables, it can in principle be tackled with any existing local or global optimization algorithm. The focus in the next subsection is on spatial branch-and-bound.

3.3 Spatial Branch-and-Bound for Direct Single Shooting

Spatial branch-and-bound [36, 37] for direct single shooting starts with an initial partition $\mathcal{A} = \{\mathbb{A}_0\}$, where $\mathbb{A}_0 \subseteq \mathbb{R}^{n_a}$ is a compact set satisfying

$$\mathbb{A}_0 \supseteq \mathbb{D}^* := \left\{ a \in \mathbb{R}^{n_a} \,\middle|\, \forall t \in [0,T], \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t) \right\}. \tag{6}$$

Note that the set $\mathbb{D}^*$ is compact if Assumption A4 is satisfied, and therefore the branch-and-bound method can always be initialized by choosing a sufficiently large interval vector $\mathbb{A}_0$ containing the set $\mathbb{D}^*$. Branching and fathoming, the two main operations in spatial branch-and-bound are reviewed next.

Branching Operation This operation updates a nonempty partition $\mathcal{A}$ by subdividing any set $\mathbb{A} \in \mathcal{A}$ into two[1] compact subsets $\mathbb{A}_\mathrm{l}$ and $\mathbb{A}_\mathrm{r}$ with $\mathbb{A}_\mathrm{l} \cup \mathbb{A}_\mathrm{r} = \mathbb{A}$ and defining

$$\mathcal{A} \leftarrow \mathcal{A}^+ := \big(\mathcal{A} \setminus \{\mathbb{A}\}\big) \cup \{\mathbb{A}_\mathrm{l}, \mathbb{A}_\mathrm{r}\}.$$

Many heuristics can be applied for deciding which set in $\mathcal{A}$ should be subdivided in priority and how to make the subdivision—see, for instance, [38, 39]. From a theoretical standpoint, the basic requirement for convergence is that the subdivision process is exhaustive, which requires that

$$\operatorname{diam}(\mathcal{A}) := \max_{\mathbb{A}\in\mathcal{A}} \operatorname{diam}(\mathbb{A}) \to 0. \tag{7}$$

Fathoming Operation Suppose that upper and lower bounds $U_M(\mathbb{A})$ and $L_M(\mathbb{A})$ can be computed such that

$$L_M(\mathbb{A}) \le \mathcal{V}_M(\mathbb{A}) \le U_M(\mathbb{A})$$

for any compact set $\mathbb{A}$ in a nonempty partition $\mathcal{A}$. If any element $\mathbb{A} \in \mathcal{A}$ is such that

$$L_M(\mathbb{A}) = \infty \quad \text{or} \quad \exists \mathbb{A}' \in \mathcal{A}: \quad L_M(\mathbb{A}) > U_M\big(\mathbb{A}'\big),$$

then it can be safely discarded from the partition $\mathcal{A}$ by applying the fathoming operation:

$$\mathcal{A} \leftarrow \mathcal{A}^+ := \mathcal{A} \setminus \{\mathbb{A}\}.$$

It can be established [24] that the spatial branch-and-bound algorithm for direct single shooting will converge to the optimal value $\mathcal{V}_M(\mathbb{R}^{n_a})$ if the following two conditions are satisfied:

1. The subdivision process is exhaustive, that is, condition (7) is satisfied.
2. The upper and lower bounds are converging for every sequence $\mathbb{A}_1, \mathbb{A}_2, \ldots \subseteq \mathbb{R}^{n_a}$ of compact sets with $\lim_{i\to\infty} \operatorname{diam}(\mathbb{A}_i) = 0$ and $\limsup_{i\to\infty} L_M(\mathbb{A}_i) < \infty$, that is, the following condition is satisfied:

$$\lim_{i\to\infty} U_M(\mathbb{A}_i) - L_M(\mathbb{A}_i) = 0.$$

[1] In a more general implementation of the branching operation, the set $\mathbb{A}$ can be subdivided into more than two subsets. This is useful, for instance, when running the algorithm on a multiprocessor computer, thereby enabling multiple branches to be analyzed in parallel.

Algorithm 1 Computing lower and upper bounds $L_M(\mathbb{A})$ and $U_M(\mathbb{A})$ for $\mathcal{V}_M(\mathbb{A})$

Input: Compact set $\mathbb{A} \in \mathcal{A}$.

Algorithm:

1. If $\mathbb{A} \cap \mathbb{D}^* = \varnothing$, return $L_M(\mathbb{A}) = U_M(\mathbb{A}) = \infty$.
2. Compute compact inner and outer approximations $\underline{\mathbb{Y}}(t, \mathbb{A}), \overline{\mathbb{Y}}(t, \mathbb{A}) \subseteq \mathbb{R}^{n_x}$ such that

$$\forall t \in [0, T], \quad \underline{\mathbb{Y}}(t, \mathbb{A}) \subseteq \bigcup_{a \in \mathbb{A}} \{y(t, a)\} \subseteq \overline{\mathbb{Y}}(t, \mathbb{A}).$$

3. If there exists $t \in [0, T]$ with $\overline{\mathbb{Y}}(t, \mathbb{A}) \cap \mathbb{F}_x(t) = \varnothing$, return $L_M(\mathbb{A}) = \infty$ and $U_M(\mathbb{A}) = \infty$; otherwise, solve the lower-bounding problem

$$L_M(\mathbb{A}) = \min_y \Psi(y) \quad \text{s.t.} \quad y \in \overline{\mathbb{Y}}(T, \mathbb{A}).$$

4. If $\underline{\mathbb{Y}}(t, \mathbb{A}) \subseteq \mathbb{F}_x(t)$ for all $t \in [0, T]$, solve the upper-bounding problem

$$U_M(\mathbb{A}) = \min_y \Psi(y) \quad \text{s.t.} \quad y \in \underline{\mathbb{Y}}(T, \mathbb{A});$$

   otherwise, return $U_M(\mathbb{A}) = \infty$.

Output: Lower and upper bounds $L_M(\mathbb{A}) \le \mathcal{V}_M(\mathbb{A}) \le U_M(\mathbb{A})$.

It is common practice to interrupt the spatial branch-and-bound algorithm as soon as the condition

$$\min_{\mathbb{A} \in \mathcal{A}} \{U_M(\mathbb{A})\} - \min_{\mathbb{A} \in \mathcal{A}} \{L_M(\mathbb{A})\} \le \varepsilon$$

is met for a desired finite accuracy $\varepsilon > 0$, hence providing so-called ε-suboptimal solutions of problem (4) after a finite number of branch-and-bound iterations.

3.4 Lower and Upper Bounding Strategy for Direct Single Shooting

For a given compact set $\mathbb{A}$, a lower bound $L_M(\mathbb{A})$ and an upper bound $U_M(\mathbb{A})$ on the optimal value $\mathcal{V}_M(\mathbb{A})$ can be found using Algorithm 1. Note that these bounds can be either finite or infinite.

A number of comments are in order regarding the steps in Algorithm 1.

- In Step 1, computing the set $\mathbb{D}^*$ as defined in (6) involves checking a semi-infinite inequality of the form

$$\forall t \in [0, T], \quad \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t).$$

  Although a hard problem in general, this semi-infinite inequality can be rewritten equivalently as a linear matrix inequality (LMI) in the coefficients $a_0, \ldots, a_M$

when the Φ_is are polynomial functions and the sets $\mathbb{F}_u(t)$ are intervals, e.g., by using the sum-of-squares approach [40]. This way, the feasibility check can be performed using efficient convex optimization techniques.

- A major difficulty in Step 2 is the computation of the outer-approximation function $\overline{\mathbb{Y}}(\cdot, \mathbb{A})$ on the solution set of the parametric ODE (3) on $[0, T]$. The quality of such enclosure functions contributes significantly to the performance of the branch-and-bound algorithm, as poor state bounds generally lead to an explosion in the size of the partition $\mathcal{A}$. Major differences between the existing techniques for global optimal control based on direct single shooting are in the way these bounds are generated. In [21], the state bounds are obtained based on the theory of differential inequalities [41]. In contrast, pointwise-in-time, convex and concave bounds on the parametric ODE solutions are considered in [42–45] based on the McCormick relaxation technique [46]. In another approach, interval enclosures are derived from a Taylor model of the parametric ODE solutions [20, 47, 48]. This latter approach was recently extended to enable convex and concave bounds in [49] using so-called McCormick–Taylor models [50]. The computation of guaranteed state bounds has also been considered in different contexts, including reachability analysis and robust control [51–53]. In principle, such ellipsoidal bounds could be used in global optimal control methods too, although there seems to be no literature on this yet. We also note that, in order for the branch-and-bound algorithm to converge, the enclosures $\overline{\mathbb{Y}}(t, \mathbb{A})$ must be convergent, i.e.,

$$\lim_{i\to\infty} \operatorname{diam}\bigl(\overline{\mathbb{Y}}(t, \mathbb{A}_i)\bigr) = 0 \tag{8}$$

for all $t \in [0, T]$ and for all sequences $\mathbb{A}_1, \mathbb{A}_2, \ldots \subseteq \mathbb{R}^{n_a}$ of compact sets such that $\lim_{i\to\infty} \operatorname{diam}(\mathbb{A}_i) = 0$ and $\limsup_{i\to\infty} L_M(\mathbb{A}_i) < \infty$.
- The computation of inner-approximation functions $\underline{\mathbb{Y}}(\cdot, \mathbb{A})$ on the solution set of the parametric ODE (3) on $[0, T]$ presents less difficulty than $\overline{\mathbb{Y}}(\cdot, \mathbb{A})$. One such function can always be obtained as

$$\underline{\mathbb{Y}}(t, \mathbb{A}) = \bigl\{y\bigl(t, \operatorname{mid}(\mathbb{A})\bigr)\bigr\}.$$

In another variant, a feasible point or a local minimizer of the single-shooting problem (4) can be sought by linking to a suitable (local) optimal control solver, and this solution point can then be used to construct $\underline{\mathbb{Y}}(t, \mathbb{A})$ instead of $\operatorname{mid}(\mathbb{A})$ in (8). Multiple points in $\mathbb{A}$ could be used to construct the inner-approximation sets $\underline{\mathbb{Y}}(t, \mathbb{A})$ likewise. Note that all of these variants satisfy the condition that

$$\lim_{i\to\infty} \operatorname{diam}\bigl(\underline{\mathbb{Y}}(t, \mathbb{A}_i)\bigr) = 0$$

for all $t \in [0, T]$ and for all sequences $\mathbb{A}_1, \mathbb{A}_2, \ldots \subseteq \mathbb{R}^{n_a}$ of compact sets such that $\lim_{i\to\infty} \operatorname{diam}(\mathbb{A}_i) = 0$.
- The minimization problems in Steps 3 and 4 are nonconvex in general. Various strategies have been developed, which determine a convergent lower bound $L_M(\mathbb{A})$ without the need for solving this optimization problem exactly. This includes interval analysis and constraint propagation [54, 55]; an extension of the αBB method [56] through the use of second-order state sensitivity and/or adjoint information

[21, 57], McCormick's relaxation technique [17, 22, 58], and, more recently, polyhedral relaxations from Taylor or McCormick–Taylor models [23]. Depending on the expression of the sets $\mathbb{F}_x(t)$, the feasibility checks that are part of Steps 3 and 4 may be nontrivial to implement as well. We refer the reader to [59–61] for a discussion of reliable strategies for the determination and verification of feasible points.

A major shortcoming of direct single shooting and its variants for global optimal control is that no guarantee can be provided on the error $(\mathcal{V}_M(\mathbb{R}^{n_a}) - \mathcal{V})$ introduced by the control parameterization in general. In other words, while ε-optimality can be guaranteed for the discretized NLP problem (4), this is not the case for the original optimal control problem (1). In principle, it is of course possible to progressively refine the control parameterization, but then the lower bounding problems have to be reconstructed ab initio every time. This quickly becomes computationally intractable within a standard branch-and-bound approach, especially when the domain of the decision variables is large. Moreover, a lower bound on the actual optimal value $\mathcal{V}$ cannot be determined with this naïve refinement approach. A principal aim of the bounding techniques and branch-and-lift algorithm developed in the following sections is to address these shortcomings.

4 Image of the Control Parameterization Error in the State Space

This section aims at examining the response mismatch that is associated with a given parameterization a of the control input u. Specifically, we compare the solution $y(t,a)$ of the parametric ODE (3) with the solution $x(t,u)$ of the original ODE

$$\forall t \in [0,T], \quad \dot{x}(t,u) = f\big(x(t,u)\big) + G\big(x(t,u)\big)u(t), \quad \text{with} \quad x(0,u) = x_0. \tag{9}$$

In this notation, the state vector $x(t,\cdot): L^2[0,T]^{n_u} \to \mathbb{R}^{n_x}$ is regarded as a functional of the control input u, defined implicitly as the solution of the ODE (9). In order to analyze the difference between $x(t,u)$ and $y(t,a)$, we start by defining the set of admissible controls associated with a parameterization $a \in \mathbb{R}^{n_a}$ as

$$\mathbb{U}_M(a) := \left\{ u \in L^2[0,T]^{n_u} \;\middle|\; \begin{array}{ll} a_i = \frac{1}{\sigma_i}\langle u, \Phi_i\rangle_\mu & \forall i \in \{0,\ldots,M\} \\ u(t) \in \mathbb{F}_u(t) & \forall t \in [0,T] \end{array} \right\}. \tag{10}$$

We also define the domain $\mathbb{D}_M \subseteq \mathbb{R}^{n_a}$ of $\mathbb{U}_M$ as

$$\mathbb{D}_M := \big\{ a \in \mathbb{R}^{n_a} \mid \mathbb{U}_M(a) \neq \varnothing \big\}.$$

The following definition makes use of this notation.

Definition 4.1 The set-valued function $\mathbb{E}_M : [0,T] \times \mathbb{D}_M \to \mathcal{P}(\mathbb{R}^{n_x})$, with $M \geq 0$, given by

$$\forall (t,a) \in [0,T] \times \mathbb{D}_M, \quad \mathbb{E}_M(t,a) := \big\{ x(t,u) - y(t,a) \mid u \in \mathbb{U}_M(a) \big\},$$

is called the *image of the control parameterization error in the state space*.

At this point, it is worth recalling that the solution trajectories x and y of the ODEs (3) and (9) are guaranteed to exist and to be unique for all possible choices of $a \in \mathbb{D}_M$ and all feasible control inputs u according to the blanket Assumption A2. Therefore, the sets $\mathbb{E}_M(\cdot, a)$ are well defined. The following proposition is merely a reinterpretation of Definition 4.1.

Proposition 4.1 *Let $u \in L^2[0,T]^{n_u}$ with $u(t) \in \mathbb{F}_u(t)$ for all $t \in [0,T]$, and let $M \geq 0$. The response $x(t,u)$ of the original ODE (9) with input function u is bounded as*

$$\forall t \in [0,T], \quad x(t,u) \in \left\{y(t,a)\right\} \oplus \mathbb{E}_M(t,a),$$

with $a_i = \frac{1}{\sigma_i}\langle u, \Phi_i\rangle_\mu$ for all $i \in \{0,\dots,M\}$.

The image set $\mathbb{E}_M$ is illustrated in a simple example next.

Example 4.1 Consider the scalar ODE $\dot{x}(t) = u(t)$ with initial condition $x(0) = 0$, $T = 1$, and $\mathbb{F}_u(t) = [-1,1]$. For simplicity, consider the constant control parameterization $\Phi_0(t) = 1$ with $\mu(t) = 1$, $\sigma_0 = 1$, and $M = 0$. The construction of an explicit representation of the image set $\mathbb{E}_0(t,a_0)$ proceeds as follows:

1. The set $\mathbb{U}_0(a_0)$ takes the form

$$\forall a_0 \in \mathbb{R}, \quad \mathbb{U}_0(a_0) = \left\{ u \in L^2[0,T]^{n_u} \,\middle|\, \begin{array}{ll} a_0 = \int_0^1 u(t)\,\mathrm{d}t & \\ -1 \leq u(t) \leq 1 & \text{for all } t \in [0,t] \end{array} \right\}. \tag{11}$$

   Since the average value of a function whose range is enclosed in $[-1,1]$ is itself in $[-1,1]$, we have $\mathbb{U}_0(a_0) = \varnothing$ for all a_0 with $|a_0| > 1$, and it follows that $\mathbb{D}_0 = [-1,1]$.
2. Consider the special case that $a_0 = 1$. It follows from (11) that the set $\mathbb{U}_0(1)$ is comprised of all functions $u \in L^2[0,T]^1$ such that $u(t) \in [-1,1]$ for all $t \in [0,1]$ and $u(t) = 1$ for almost all $t \in [0,1]$. Thus, for all $u \in \mathbb{U}_0(1)$, we have

$$\forall t \in [0,1], \quad x(t,u) = \int_0^t u(t)\,\mathrm{d}t = t.$$

   Since $y(t,1) = a_0 t = t$, we obtain $\mathbb{E}_0(t,1) = \{0\}$ for all $t \in [0,1]$. By a similar argument, it is shown that $\mathbb{E}_0(t,-1) = \{0\}$ for all $t \in [0,1]$.
3. Before discussing the general case, consider the sets $\mathbb{E}_0(t,a_0)$ for $a_0 \in [-1,1]$ and $t = 1$. Since $y(1,a_0) = a_0$ and

$$\forall u \in \mathbb{U}_0(a_0), \quad x(1,u) = \int_0^1 u(t)\,\mathrm{d}t = a_0,$$

   we have $\mathbb{E}_0(1,a_0) = \{0\}$ for all $a_0 \in [-1,1]$.

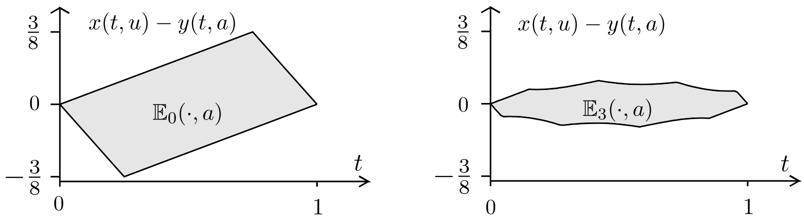

Fig. 1 *Left*: Image set $\mathbb{E}_0(\cdot,a)$ on $[0,1]$ for $a=\frac{1}{2}$ as introduced in Example 4.1. *Right*: Image set $\mathbb{E}_3(\cdot,a)$ on $[0,1]$ for $a=(\frac{1}{2},0,0)^\mathsf{T}$ for the same example illustrating that the diameter of the set $\mathbb{E}_M(t,a)$ shrinks for increasing M (see Theorem 4.1)

4. Finally, consider the general solution set $\mathbb{E}_0(t,a_0)$ for any given $a_0\in[-1,1]$ and any $t\in[0,1]$. Since the ODE is linear and the sets $\mathbb{F}_u(t):=[-1,1]$ are convex, it follows that the sets $\mathbb{U}_0(a_0)$ and $\mathbb{E}_0(t,a_0)$ are themselves convex at each $t\in[0,1]$. Consequently, $\mathbb{E}_0(t,a_0)$ is an interval with lower and upper bounds $E_0^{\mathrm{L}}(t,a_0)$, $E_0^{\mathrm{U}}(t,a_0)$ given by

$$E_0^{\mathrm{L/U}}(t,a_0)=\min_u/\max_u\int_0^t u(t)\,\mathrm{d}t-a_0t\quad\text{s.t.}\quad\begin{cases}\int_0^1 u(t)\,\mathrm{d}t=a_0,\\ -1\le u(t)\le 1.\end{cases}$$

These linear optimization problems can be solved explicitly by applying Pontryagin's maximum principle, giving:

$$\forall(a_0,t)\in[0,1]\times[0,T],$$

$$\mathbb{E}_0(t,a_0)=\begin{cases}[-(1+a_0)t,(1-a_0)t] & \text{if } t\in[0,\frac{1-a_0}{2}],\\ [-(1-a_0)(1-t),(1-a_0)t] & \text{if } t\in]\frac{1-a_0}{2},\frac{1+a_0}{2}[,\\ [-(1-a_0)(1-t),(1+a_0)(1-t)] & \text{if } t\in[\frac{1+a_0}{2},1];\end{cases}$$

$$\forall(a_0,t)\in[-1,0]\times[0,T],$$

$$\mathbb{E}_0(t,a_0)=\begin{cases}[-(1+a_0)t,(1-a_0)t] & \text{if } t\in[0,\frac{1+a_0}{2}],\\ [-(1+a_0)t,(1+a_0)(1-t)] & \text{if } t\in]\frac{1+a_0}{2},\frac{1-a_0}{2}[,\\ [-(1-a_0)(1-t),(1+a_0)(1-t)] & \text{if } t\in[\frac{1-a_0}{2},1].\end{cases}$$

The left plot on Fig. 1 represents the set $\mathbb{E}_0(t,a_0)$ for $a_0=\frac{1}{2}$.

In general, explicit and exact characterizations of the image sets $\mathbb{E}_M(t,a)$ cannot be obtained as in Example 4.1. Instead, conservative approximations for these sets are sought, which can be characterized explicitly and in a computationally tractable way. We start by noting that, under the blanket Assumptions A2 and A4, the sets $\mathbb{E}_M(t,a)$ are compact [62]. The following additional assumption concerns the family of orthogonal basis functions $\{\Phi_i\}_{i\in\mathbb{N}}$.

Assumption 4.1 *The functions $\{\Phi_i\}_{i\in\mathbb{N}}$ are smooth and define an orthogonal basis on $[0,T]$ with respect to the weighting function μ and the scaling factors $\{\sigma_i\}_{i\in\mathbb{N}}$ such* *that* $\sum_{i=0}^{\infty} \sigma_i = \infty$. *Moreover, for any piecewise smooth function* $\omega : [0, T] \to \mathbb{R}$, *there exist constants* $C_\omega^0 \in \mathbb{R}$ *and* $C_\omega^1 \in \mathbb{R}_{++}$, *together with a sequence of functions* $\varphi_1, \varphi_2, \ldots \in L^2[0, T]$ *with* $\varphi_M \in \operatorname{span}(\Phi_1, \ldots, \Phi_M)$ *for all* $M \in \mathbb{N}$, *such that*

$$\forall M \in \mathbb{N}, \quad \log\bigl(\bigl|\omega(t) - \varphi_M(t)\bigr|\bigr) \le C_\omega^0 - C_\omega^1 M \tag{12}$$

for almost all $t \in [0, T]$.

Remark 4.1 One way to construct orthogonal basis functions $\{\Phi_i\}_{i\in\mathbb{N}}$ on $[0, T]$ that satisfy Assumption 4.1 is by applying a Gram–Schmidt process to the monomial function basis $\{1, x, x^2, \ldots\}$. This yields the Legendre polynomials

$$\forall i \in \mathbb{N}, \quad \Phi_i(t) = (-1)^i \sum_{j=0}^{i} \binom{i}{j} \binom{i+j}{j} \left(-\frac{t}{T}\right)^j,$$

which are orthogonal with respect to the unit measure $\mu(t) = 1$. The associated scaling factors are $\sigma_i := \frac{T}{2i+1}$ and satisfy $\sum_{i=0}^{\infty} \sigma_i = \infty$, as required by Assumption 4.1. Although we keep our considerations general in deriving the theoretical results, Legendre polynomials present many computational advantages and are the method of choice for control parameterization here.

Example 4.1 (Continued) The right plot on Fig. 1 represents the set $\mathbb{E}_3(t, a)$ at $a = (\frac{1}{2}, 0, 0)$ for the same differential equation and control constraints as in Example 4.1, using the first three Legendre polynomials Φ_0, Φ_1, and Φ_2.

Remark 4.2 The exponential convergence condition (12) holds for any orthogonal polynomial basis since for any given piecewise smooth function $\omega : [0, T] \to \mathbb{R}$, there exists a sequence of polynomials which approximate ω with exponentially converging accuracy, as proven in [63]. The exponential convergence condition (12) can also be established in the case of trigonometric Fourier expansions [64].

Before stating the main result of this section, we discuss a technical detail, namely the need to introduce the condition $\sum_{i=0}^{\infty} \sigma_i = \infty$ for the sequence $\{\sigma_i\}_{i\in\mathbb{N}}$ in Assumption 4.1.

Lemma 4.1 *Let Assumption* 4.1 *and the blanket Assumption* A4 *be satisfied. Then, there exists a constant* $\alpha < \infty$ *such that* $\|a_i\|_\infty < \alpha$ *for all* $i \in \mathbb{N}$ *and for all* $a \in \mathbb{D}_\infty$.

Proof Since $\mathbb{F}_u(t)$ is compact (Assumption A4), there exists a constant $\gamma < \infty$ such that $\langle u_j, u_j \rangle_\mu \le \gamma$ for all L^2-integrable u with $u(t) \in \mathbb{F}_u(t)$ and all $j \in \{1, \ldots, n_u\}$. By contradiction, assume that there exists a sequence $a \in \mathbb{D}_\infty$ for which $\limsup_{i\to\infty} |(a_i)_j| \ne 0$. Since $\sum_{i=0}^{\infty} \sigma_i = \infty$ (Assumption 4.1), Bessel's inequality (see Proposition 3.1) gives

$$\infty = \sum_{i=0}^{\infty} \bigl|(a_i)_j\bigr|^2 \sigma_i \le \langle u_j, u_j \rangle_\mu \le \gamma < \infty$$

for any $u \in \mathbb{U}_\infty(a)$, which is a contradiction. Therefore, we have $\limsup_{i\to\infty} |(a_i)_j| = 0$, and there exists an upper bound $\alpha < \infty$ such that $\|a_i\|_\infty < \alpha$ for all $i \in \mathbb{N}$ and all coefficient sequences $a \in \mathbb{D}_\infty$. □

The following theorem provides a condition under which $\mathbb{E}_M(t,a)$ converges to $\{0\}$ as $M \to \infty$. A proof of this theorem is given and discussed in Appendix A.

Theorem 4.1 *Let Assumption 4.1 and the blanket Assumptions* A2 *and* A4 *be satisfied. Then, there exist constants $C_E^0 \in \mathbb{R}$ and $C_E^1 \in \mathbb{R}_{++}$ such that the condition*

$$\forall a \in \mathbb{D}_M, \quad \log\bigl(\operatorname{diam}(\mathbb{E}_M(t,a))\bigr) \le C_E^0 - C_E^1 M$$

is satisfied for all $M \in \mathbb{N}$ and for all $t \in [0,T]$.

A major implication of Theorem 4.1 is that, for any sequence $a \in \mathbb{D}_\infty$, the associated sequence of image sets satisfies

$$\forall t \in [0,T], \quad \lim_{M\to\infty} \mathbb{E}_M\bigl(t, \bigl(a_0^\mathsf{T}, \dots, a_M^\mathsf{T}\bigr)^\mathsf{T}\bigr) = \{0\}.$$

Nonetheless, this convergence property of the image set relies crucially on the assumption that the right-hand side of the ODE is affine in u. This property is not satisfied, in general, by those dynamic systems that are nonlinear in the control input u, as illustrated in the following example.

Example 4.2 Consider the scalar ODE $\dot{x}(t) = u(t)^2$ with initial condition $x(0) = 0$ and $\mathbb{F}_u(t) = [-1, 1]$. For any $M \ge 0$, the image of the control parameterization error at $a_0 = \cdots = a_M = 0$ is given by

$$\forall t \in [0,T], \quad \mathbb{E}_M(t,0) = \left\{ \int_0^t u(\tau)^2 \, \mathrm{d}\tau \mid u \in \mathbb{U}_M(0) \right\} = [0,t].$$

The right-most equality follows from the fact that, for any order $M \ge 0$, the set $\mathbb{U}_M(0)$ contains bang-bang control functions u with $u(t) \in \{-1, 1\}$ for which $x(t) = t$. Consequently, we have $\lim_{M\to\infty} \mathbb{E}_M(t,0) \supsetneq \{0\}$ for $t > 0$.

5 Spatial Branch-and-Lift Algorithm for Global Optimal Control

This section presents the branch-and-lift algorithm, which builds upon a generic, spatial branch-and-bound algorithm and is rigorous in its accounting of the control parameterization error. The basic idea is to bracket the solution of the original optimal control problem and progressively refine these bounds via a lifting mechanism that increases the control parameterization order.

In order to describe the algorithm, it is useful to consider for any compact and finite-dimensional coefficient set $\mathbb{A} \subseteq \mathbb{R}^{n_a}$ an auxiliary (infinite-dimensional) optimal control problem of the form

$$\mathcal{V}_M^*(\mathbb{A}) := \min_u \Psi\bigl(x(T,u)\bigr) \quad \text{s.t.} \quad \begin{cases} x(t,u) \in \mathbb{F}_x(t), & \forall t \in [0,T], \\ u \in \mathbb{U}_M(\mathbb{A}). \end{cases} \tag{13}$$

Here, $\mathbb{U}_M(\mathbb{A}) := \bigcup_{a\in\mathbb{A}} \mathbb{U}_M(a)$ stands for the set of all control functions $u \in L^2[0,T]^{n_u}$ that satisfy the control constraints $u(t) \in \mathbb{F}_u(t)$ for all $t \in [0,T]$, as well as the condition

$$\left(\frac{1}{\sigma_0}\langle u, \Phi_0\rangle_\mu^\mathsf{T}, \ldots, \frac{1}{\sigma_M}\langle u, \Phi_M\rangle_\mu^\mathsf{T}\right)^\mathsf{T} \in \mathbb{A}.$$

The following properties are readily verified:

P1. $\mathcal{V}_M^*(\mathbb{A}) \geq \mathcal{V}$ for all $\mathbb{A} \subseteq \mathbb{R}^{n_a}$, that is, $\mathcal{V}_M^*(\mathbb{A})$ yields an upper bound on the optimal value $\mathcal{V}$ of problem (1).

P2. There exists a global optimizer u^* of problem (1) whose $M+1$ first Gram–Schmidt coefficients are in the set $\mathbb{A} \subseteq \mathbb{R}^{n_a}$ if and only if $\mathcal{V}_M^*(\mathbb{A}) = \mathcal{V} < \infty$.

Remark 5.1 The key difference between the optimal value functions $\mathcal{V}_M^*$ of problem (13) and the optimal value functions $\mathcal{V}_M$ of the single-shooting approximation in problem (4) is that $\mathcal{V}_M^*(\mathbb{R}^{n_a}) = \mathcal{V}$, whereas $\mathcal{V}_M(\mathbb{R}^{n_a}) \neq \mathcal{V}$ in general.

Procedures for computing lower and upper bounds on $\mathcal{V}_M^*(\mathbb{A})$ are described next (Sect. 5.1), before introducing the new lifting step (Sect. 5.2) and its integration within branch-and-bound search (Sect. 5.3) as well as discussing convergence aspects (Sect. 5.4).

5.1 Lower- and Upper-Bounding Procedures

This section aims at deriving lower and upper bounds on the optimal value $\mathcal{V}_M^*(\mathbb{A})$ of the optimal control problem (13). The idea is to approximate the state $x(t,u)$ with the parametric function $y(t,a)$ and at the same time keep track of the parameterization error. Specifically, we use the image sets $\mathbb{E}_M(t,a)$ defined in Sect. 4 in order to define relaxed and tightened feasible sets $\overline{\mathbb{F}}_M(t,a)$ and $\underline{\mathbb{F}}_M(t,a)$, respectively, as

$$\forall t \in [0,T], \quad \overline{\mathbb{F}}_M(t,a) := \mathbb{F}_x(t) \oplus \mathbb{E}_M(t,a), \quad \text{and}$$

$$\forall t \in [0,T], \quad \underline{\mathbb{F}}_M(t,a) := \mathbb{F}_x(t) \ominus \mathbb{E}_M(t,a).$$

In turn, auxiliary, finite-dimensional optimization problems can be stated as

$$\underline{\mathcal{V}}_M(\mathbb{A}) := \min_a \min_{e\in\mathbb{E}_M(T,a)} \Psi\big(y(T,a)+e\big) \tag{14}$$
$$\text{s.t.} \quad \begin{cases} y(t,a) \in \overline{\mathbb{F}}_M(t,a) & \forall t \in [0,T], \\ a \in \mathbb{A} \cap \mathbb{D}_M, \end{cases}$$

$$\overline{\mathcal{V}}_M(\mathbb{A}) := \min_a \max_{e\in\mathbb{E}_M(T,a)} \Psi\big(y(T,a)+e\big) \tag{15}$$
$$\text{s.t.} \quad \begin{cases} y(t,a) \in \underline{\mathbb{F}}_M(t,a) & \forall t \in [0,T], \\ a \in \mathbb{A} \cap \mathbb{D}_M. \end{cases}$$

These auxiliary optimization problems enjoy the following property by construction.

Proposition 5.1 *The inequality* $\underline{\mathcal{V}}_M(\mathbb{A}) \le \mathcal{V}_M^*(\mathbb{A}) \le \overline{\mathcal{V}}_M(\mathbb{A})$ *holds for all compact sets* $\mathbb{A} \subseteq \mathbb{R}^{n_a}$ *and for all* $M \in \mathbb{N}$.

Proof Let $u^* \in \mathbb{U}_M(\mathbb{A})$ be a minimizer of the optimal control problem (13), so that $\mathcal{V}_M^*(\mathbb{A}) = \Psi(x(T,u^*))$ and $x(t,u^*) \in \mathbb{F}_x(t)$ for all $t \in [0,T]$. Define the coefficients $a_i^* := \langle u^*, \Phi_i\rangle_\mu$ for all $i \in \{0,\dots,M\}$, so that $a^* \in \mathbb{A}$, as well as the response defect $d^*(t) := x(t,u^*) - y(t,a^*)$. It follows from the definitions of the sets $\mathbb{U}_M(\mathbb{A})$ and $\mathbb{E}_M(t,a^*)$ that

$$\begin{aligned}\mathcal{V}_M^*(\mathbb{A}) &= \Psi\big(x\big(T,u^*\big)\big) = \Psi\big(y\big(T,a^*\big) + d^*(T)\big) \quad \text{and}\\ y\big(t,a^*\big) &\in \mathbb{F}_x(t) \oplus \mathbb{E}_M\big(t,a^*\big).\end{aligned}$$

Therefore, the pair $(a^*, d^*(T))$ is a feasible point of the optimal control problem (14), and we have

$$\underline{\mathcal{V}}_M(\mathbb{A}) \le \Psi\big(y\big(T,a^*\big) + d^*(T)\big) = \mathcal{V}_M^*(\mathbb{A}).$$

Concerning the upper-bounding part, if the pair (a^*, e^*) is an optimizer (min-max point) of problem (15), then there exists a function $u^* \in \mathbb{U}_M(a^*)$ with $y(T,a^*) + e^* = x(T,u^*)$. Since $y(t,a^*) \in \mathbb{F}_x(t) \ominus \mathbb{E}_M(t,a^*)$ for all $t \in [0,T]$, we have that any function $u^* \in \mathbb{U}_M(a^*)$ satisfies $x(t,u^*) \in \mathbb{F}_x(t)$ for all $t \in [0,T]$. Therefore, u^* is a feasible point of problem (13), and it follows that

$$\mathcal{V}_M^*(\mathbb{A}) \le \Psi\big(x\big(t,u^*\big)\big) = \Psi\big(y\big(t,a^*\big) + e^*\big) = \overline{\mathcal{V}}_M(\mathbb{A}). \qquad \square$$

Remark 5.2 The right-hand inequality $\mathcal{V}_M^*(\mathbb{A}) \le \overline{\mathcal{V}}_M(\mathbb{A})$ in Proposition 5.1 could be tightened by replacing the inner maximization problem in (15) with a minimization problem. The reason for using (15) here is because only a conservative enclosure of $\mathbb{E}_M(T,a)$ can be computed in practice, instead of the exact set $\mathbb{E}_M(T,a)$.

In general, direct solution of the optimal control problems (14) and (15) is not possible since an exact characterization of $\mathbb{E}_M$ is typically unavailable. Instead, lower and upper bounds $\overline{U}_M(\mathbb{A}) \ge \overline{\mathcal{V}}_M(\mathbb{A})$ and $\underline{L}_M(\mathbb{A}) \le \underline{\mathcal{V}}_M(\mathbb{A})$ are sought in order to make the problem computationally tractable. A procedure for computing such bounds is presented in Algorithm 2. This procedure relies on the generic capability to compute enclosure functions $\underline{\mathbb{Y}}(t,\mathbb{A}), \overline{\mathbb{Y}}(t,\mathbb{A}) \subseteq \mathbb{R}^{n_x}$ and $\overline{\mathbb{E}}_M(t,\mathbb{A}) \subseteq \mathbb{R}^{n_x}$ for every compact set $\mathbb{A} \subset \mathbb{R}^{n_a}$, which satisfy

$$\begin{aligned}&\forall t \in [0,T],\\ &\underline{\mathbb{Y}}(t,\mathbb{A}) \subseteq \bigcup_{a\in\mathbb{A}} \big\{y(t,a)\big\} \subseteq \overline{\mathbb{Y}}(t,\mathbb{A}) \quad \text{and} \quad \bigcup_{a\in\mathbb{A}} \mathbb{E}_M(t,a) \subseteq \overline{\mathbb{E}}_M(t,\mathbb{A}).\end{aligned}$$

Methods and tools to generate the enclosure functions $\underline{\mathbb{Y}}(\cdot,\mathbb{A})$ and $\overline{\mathbb{Y}}(\cdot,\mathbb{A})$ have been discussed earlier in connection with direct single shooting (Sect. 3.4) and Algorithm 1. Computing the enclosure functions $\overline{\mathbb{E}}_M(\cdot,\mathbb{A})$ can be rather involved too, and one possible approach based on ellipsoidal techniques is discussed in Appendix B.

Algorithm 2 Computing lower and upper bounds $\underline{L}_M(\mathbb{A})$ and $\overline{U}_M(\mathbb{A})$ for $\mathcal{V}_M^*(\mathbb{A})$

Input: Compact set $\mathbb{A} \in \mathcal{A}$.

Algorithm:

1. If $\mathbb{A} \cap \mathbb{D}_M = \varnothing$, return $\underline{L}_M(\mathbb{A}) = \overline{U}_M(\mathbb{A}) = \infty$.
2. Compute compact inner- and outer-approximations $\underline{\mathbb{Y}}(t,\mathbb{A})$ and $\overline{\mathbb{Y}}(t,\mathbb{A})$ and an enclosure $\overline{\mathbb{E}}_M(t,\mathbb{A})$ such that
$$\forall t \in [0,T],$$
$$\underline{\mathbb{Y}}(t,\mathbb{A}) \subseteq \bigcup_{a\in\mathbb{A}} \bigl\{y(t,a)\bigr\} \subseteq \overline{\mathbb{Y}}(t,\mathbb{A}) \quad \text{and} \quad \bigcup_{a\in\mathbb{A}} \mathbb{E}_M(t,a) \subseteq \overline{\mathbb{E}}_M(t,\mathbb{A}).$$
3. If there exists $t \in [0,T]$ with $\overline{\mathbb{Y}}(t,\mathbb{A}) \cap (\mathbb{F}_x(t) \oplus \overline{\mathbb{E}}_M(t,\mathbb{A})) = \varnothing$, return $\underline{L}_M(\mathbb{A}) = \overline{U}_M(\mathbb{A}) = \infty$; otherwise, solve the lower-bounding problem
$$\underline{L}_M(\mathbb{A}) := \min_y \min_e \ \Psi(y+e) \quad \text{s.t.} \quad y \in \overline{\mathbb{Y}}(T,\mathbb{A}), \quad e \in \overline{\mathbb{E}}_M(T,\mathbb{A}).$$
4. If $\underline{\mathbb{Y}}(t,\mathbb{A}) \subseteq \mathbb{F}_x(t) \ominus \overline{\mathbb{E}}_M(t,\mathbb{A})$ for all $t \in [0,T]$, solve the upper-bounding problem
$$\overline{U}_M(\mathbb{A}) := \min_y \max_e \Psi(y+e) \quad \text{s.t.} \quad y \in \underline{\mathbb{Y}}(T,\mathbb{A}), \quad e \in \overline{\mathbb{E}}_M(T,\mathbb{A});$$
otherwise, return $\overline{U}_M(\mathbb{A}) = \infty$.

Output: Lower and upper bounds $\underline{L}_M(\mathbb{A}) \le \mathcal{V}_M^*(\mathbb{A}) \le \overline{U}_M(\mathbb{A})$.

5.2 Lifting Operation

Similar to the spatial branch-and-bound algorithm described in Sect. 3.3, the proposed branch-and-lift algorithm updates a partition $\mathcal{A} := \{\mathbb{A}_1, \ldots, \mathbb{A}_k\}$ of sets $\mathbb{A}_1, \ldots, \mathbb{A}_k \subseteq \mathbb{R}^{n_a}$ by applying branching and fathoming operations. In addition, the branch-and-lift algorithm increases the control parameterization order M during the search using a new type of operation, called *lifting*.

Given a control parameterization order $M \ge 0$ and an associated a partition $\mathcal{A} = \{\mathbb{A}_1, \ldots, \mathbb{A}_k\}$, the lifting operation constructs a new partition

$$\mathcal{A} \leftarrow \mathcal{A}^+ := \bigl\{\mathbb{A}_1^+, \mathbb{A}_2^+, \ldots, \mathbb{A}_k^+\bigr\} \tag{16}$$

by increasing the dimension $M \leftarrow M^+ := M+1$. The lifted sets $\mathbb{A}_i^+$, $i = 1, \ldots, k$, are defined as

$$\mathbb{A}_i^+ := \left\{ \left(a_0^\mathsf{T}, \ldots, a_M^\mathsf{T}, a_{M+1}^\mathsf{T}\right)^\mathsf{T} \,\middle|\, \begin{array}{l} \left(a_0^\mathsf{T}, \ldots, a_M^\mathsf{T}\right)^\mathsf{T} \in \mathbb{A}_i \\ a_{M+1} \in \left[\underline{a}_{M+1}(\mathbb{A}_i), \overline{a}_{M+1}(\mathbb{A}_i)\right] \end{array} \right\}, \tag{17}$$

with

$$\underline{a}_{M+1,j}(\mathbb{A})/\overline{a}_{M+1,j}(\mathbb{A}) = \min_u / \max_u \frac{1}{\sigma_{M+1}} \langle u_j, \Phi_{M+1} \rangle_\mu \tag{18}$$
$$\text{s.t.} \quad u \in \mathbb{U}_M(\mathbb{A}),$$

for all $j \in \{1, \ldots, n_u\}$.

Remark 5.3 The optimization problems (18) are infinite-dimensional problems and therefore difficult to solve in general. However, in the special case that the sets $\mathbb{F}_u(t)$ are interval vectors—a case that is frequently encountered in practice—these problems become linear, and methods from the field of convex optimization can be used to solve them both reliably and efficiently. In the general case, one possibility for a practical implementation consists in first bounding the sets $\mathbb{F}_u(t)$ with intervals and then solving the relaxed counterparts of (18) to obtain upper and lower bounds on $\overline{a}_{M+1,j}(\mathbb{A})$ and $\underline{a}_{M+1,j}(\mathbb{A})$, respectively.

The lifting operation is illustrated in an example next.

Example 5.1 Consider a dynamic system with a single control variable $u(t) \in \mathbb{F}_u(t) = [-1, 1]$ for $t \in [0, 1]$, and assume that a partition $\mathcal{A}$ is available for a control parameterization of order $M = 1$ based on Legendre polynomials such that

$$\mathcal{A} = \{\mathbb{A}_1, \mathbb{A}_2\} \quad \text{with} \begin{cases} \mathbb{A}_1 = [-1, -0.4] \times [0.6, 1], \\ \mathbb{A}_2 = [0.3, 1] \times [0, 0.7]. \end{cases}$$

The optimization problems (18) can be solved by using convex optimization techniques. For instance, solving

$$\underline{a}_2(\mathbb{A}_1) = \min_u \int_0^1 5\big(6t^2 - 6t + 1\big)u(t)\,\mathrm{d}t \quad \text{s.t.} \quad \begin{cases} -1 \le \int_0^1 u(t)\,\mathrm{d}t \le -0.4, \\ 0.6 \le 3\int_0^1 (2t-1)u(t)\,\mathrm{d}t \le 1, \\ u(t)^2 \le 1 \quad \text{for all } t \in [0, 1], \end{cases}$$

gives $\underline{a}_2(\mathbb{A}_1) \ge -0.87$. Likewise, the other bounds are computed as

$$\overline{a}_2(\mathbb{A}_1) \le 1.58, \quad \underline{a}_2(\mathbb{A}_2) \ge -1.88, \quad \text{and} \quad \overline{a}_2(\mathbb{A}_2) \le 1.54,$$

and the result of the lifting operation is thus given by

$$\mathcal{A}^+ = \big\{\mathbb{A}_1^+, \mathbb{A}_2^+\big\} \quad \text{with} \begin{cases} \mathbb{A}_1^+ = [-1, -0.4] \times [0.6, 1] \times [-0.87, 1.58], \\ \mathbb{A}_2^+ = [0.3, 1] \times [0, 0.7] \times [-1.88, 1.54]. \end{cases}$$

The left plot in Fig. 2 shows the original sets $\mathbb{A}_1$ and $\mathbb{A}_2$, while the right plot shows the lifted sets $\mathbb{A}_1^+$ and $\mathbb{A}_2^+$. Essentially, the lifting step uses bounds on the control parameterization coefficients a_0 and a_1 in order to determine bounds on the following coefficient a_2 in a control parameterization of order $M = 2$. Clearly, the resulting

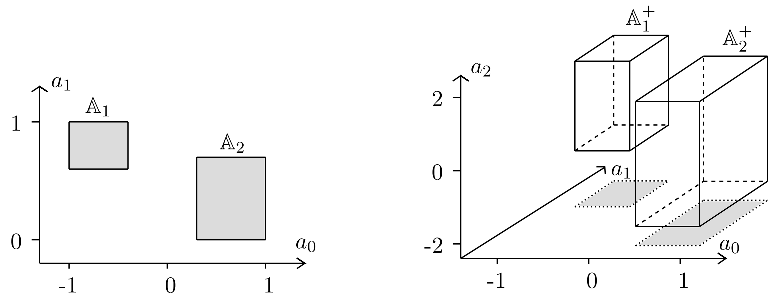

Fig. 2 Visualization of the lifting operation. *Left plot*: Sets $\mathbb{A}_1$ and $\mathbb{A}_2$ on the (a_0, a_1)-space. *Right plot*: Lifted sets $\mathbb{A}_1^+$ and $\mathbb{A}_2^+$ in the (a_0, a_1, a_2)-space

bounds on a_2 in the lifted sets $\mathbb{A}_1^+$ and $\mathbb{A}_2^+$ depend on the particular geometry of the sets $\mathbb{A}_1$ and $\mathbb{A}_2$, respectively, as well as on the geometry of the set $\mathbb{F}_u$. In this example, the width of $\mathbb{A}_1^+$ along the a_2-axis turns out to be smaller than that of $\mathbb{A}_2^+$.

The lifting step satisfies the following invariance property by construction.

Proposition 5.2 *Let $\mathbb{A}$ be a compact set and denote by $\mathbb{A}^+$ its lifted counterpart. Then, $\mathbb{U}_M(\mathbb{A}) = \mathbb{U}_{M+1}(\mathbb{A}^+)$ and, accordingly, $\mathcal{V}_M^*(\mathbb{A}) = \mathcal{V}_{M+1}^*(\mathbb{A}^+)$.*

It is important to be aware of the fact that the width of a lifted set $\mathbb{A}^+$ may be larger than the width of its parent set $\mathbb{A}$. Nonetheless, the width of the sets $\mathbb{A}$ is uniformly bounded by the constant α that was introduced in Lemma 4.1.

Proposition 5.3 *Let Assumption 4.1 and the blanket Assumption* A3 *be satisfied. Let also $\alpha < \infty$ denote the constant introduced in Lemma 4.1. Then, for any compact set $\mathbb{A}$, the width of the interval $[\overline{a}_{M+1,j}(\mathbb{A}), \underline{a}_{M+1,j}(\mathbb{A})]$ generated by a lifting operation is bounded by α, i.e., we have*

$$\forall j \in \{1, \dots, n_u\}, \quad \overline{a}_{M+1,j}(\mathbb{A}) - \underline{a}_{M+1,j}(\mathbb{A}) \le \alpha.$$

Proof The statement of the proposition follows immediately from Lemma 4.1 and by the definition of the lifting operation. □

5.3 Branch-and-Lift Algorithm

The branch-and-lift algorithm is given in Algorithm 3 and detailed subsequently. The branching and fathoming operations are the same as those defined earlier in Sect. 3.3 with the only difference that the bounds $\underline{L}_M(\mathbb{A})$ and $\overline{U}_M(\mathbb{A})$ are now used instead of $L_M(\mathbb{A})$ and $U_M(\mathbb{A})$.

Initialization The branch-and-lift algorithm starts with $M = 0$. In the case that $\Phi_0(t) = 1$, for instance, this corresponds to a constant control parameterization. The motivation here is that even a coarse parameterization might already lead to the exclusion of certain parts of the control region that cannot contain any global optima.

Algorithm 3 Branch-and-lift algorithm for global optimal control

Input: Termination tolerance $\varepsilon > 0$; Lifting parameter $\varrho > 0$

Initialization:

1. Set $M = 0$ and $\mathcal{A} = \{\mathbb{A}_0\}$, with $\mathbb{A}_0 \supseteq \mathbb{D}_0$ being an interval.

Repeat:

2. Select an interval $\mathbb{A} \in \mathcal{A}$.
3. Compute upper and lower bounds $\underline{L}_M(\mathbb{A}) \le \mathcal{V}_M^*(\mathbb{A}) \le \overline{U}_M(\mathbb{A})$ using Algorithm 2.
4. Apply a fathoming operation.
5. If $(\min_{\mathbb{A}\in\mathcal{A}} \overline{U}_M(\mathbb{A}) - \min_{\mathbb{A}\in\mathcal{A}} \underline{L}_M(\mathbb{A})) \le \varepsilon$ or $\mathcal{A} = \varnothing$, stop.
6. If the condition

$$\max_{\mathbb{A}\in\mathcal{A}} \operatorname{diam}\bigl(\overline{\mathbb{Y}}(t,\mathbb{A}) \oplus \overline{\mathbb{E}}_M(t,\mathbb{A})\bigr) \le (1+\varrho) \max_{\mathbb{A}\in\mathcal{A}} \operatorname{diam}\bigl(\overline{\mathbb{E}}_M\bigl(t, \bigl\{\operatorname{mid}(\mathbb{A})\bigr\}\bigr)\bigr)$$

holds for all $t \in [0, T]$, apply a lifting operation for $M \leftarrow M + 1$.

7. Apply a branching operation, and return to step 2.

Output: Lower and upper bounds $\min_{\mathbb{A}\in\mathcal{A}} \underline{L}_M(\mathbb{A}) \le \mathcal{V} \le \min_{\mathbb{A}\in\mathcal{A}} \overline{U}_M(\mathbb{A})$, or a proof of infeasibility.

A possible way of initializing the partition $\mathcal{A} = \{\mathbb{A}_0\}$ is by noting that the interval $[\underline{a}_0(\varnothing), \overline{a}_0(\varnothing)]$, as defined in (18), encloses all possible values of the constant parameterization coefficient a_0.

Lifting Condition Because branch-and-bound search is most efficient when the control parameterization order M is small, the branch-and-lift strategy is to increase M as infrequently as possible. Intuitively, it is desirable to apply a lifting operation whenever the error associated with the control parameterization becomes of the same order of magnitude as the reachable set of the original ODE (9) itself. The former can be evaluated as the diameter of $\overline{\mathbb{E}}_M(t, \{\operatorname{mid}(\mathbb{A})\})$ as computed at the midpoint of $\mathbb{A}$, whereas the latter can be over-approximated as the diameter of the set $\overline{\mathbb{Y}}(t,\mathbb{A}) \oplus \overline{\mathbb{E}}_M(t,\mathbb{A})$. This leads to the following lifting condition:

$$\begin{aligned} &\forall t \in [0, T], \\ &\max_{\mathbb{A}\in\mathcal{A}} \operatorname{diam}\bigl(\overline{\mathbb{Y}}(t,\mathbb{A}) \oplus \overline{\mathbb{E}}_M(t,\mathbb{A})\bigr) \le (1+\varrho) \max_{\mathbb{A}\in\mathcal{A}} \operatorname{diam}\bigl(\overline{\mathbb{E}}_M\bigl(t, \bigl\{\operatorname{mid}(\mathbb{A})\bigr\}\bigr)\bigr), \end{aligned} \tag{19}$$

where $\varrho > 0$ is a tuning parameter. Finite termination of the branch-and-lift algorithm based on the lifting condition (19) is investigated in Sect. 5.4.

In the branch-and-lift algorithm, the decision whether to perform a normal branching or to apply a lifting operation before branching based on (19) is taken at each iteration. Moreover, a lifting operation is applied *globally* to all of the parameter subsets in a current partition $\mathcal{A}$, that is, all the subsets in $\mathcal{A}$ share the same parameterization order at any iteration. As a variant of the branch-and-lift algorithm given in Algorithm 3, one could also imagine a family of subsets that would have different parameterization orders by applying the lifting condition locally instead.

5.4 Finite Termination of Branch-and-Lift Algorithm

This section aims at investigating conditions under which Algorithm 3 finds an ε-suboptimal solution of the optimal control problem (1) after a finite number of iterations. The following assumptions on the convergence of the enclosure functions $\overline{\mathbb{Y}}(t,\cdot)$ and $\overline{\mathbb{E}}_M(t,\cdot)$ are introduced to carry out the analysis.

Assumption 5.1 *There exists a constant* $C_Y < \infty$ *such that*

$$\operatorname{diam}\bigl(\overline{\mathbb{Y}}(t,\mathbb{A})\bigr) \le C_Y \operatorname{diam}(\mathbb{A}) \tag{20}$$

for all sets $\mathbb{A}$ *with a sufficiently small diameter* $\operatorname{diam}(\mathbb{A})$.

Assumption 5.2 *There exist constants* $C_{\mathbb{E}}^0 \in \mathbb{R}$, $C_{\mathbb{E}}^1 \in \mathbb{R}_{++}$, *and* $C_{\mathbb{E}}^2 \in \mathbb{R}_+$ *such that*

$$\operatorname{diam}\bigl(\overline{\mathbb{E}}_M\bigl(t,\{\operatorname{mid}(\mathbb{A})\}\bigr)\bigr) \le \exp\bigl(C_{\mathbb{E}}^0 - C_{\mathbb{E}}^1 M\bigr) \quad \textit{and} \tag{21}$$

$$\operatorname{diam}\bigl(\overline{\mathbb{E}}_M(t,\mathbb{A})\bigr) \le \operatorname{diam}\bigl(\overline{\mathbb{E}}_M\bigl(t,\{\operatorname{mid}(\mathbb{A})\}\bigr)\bigr) + C_{\mathbb{E}}^2 \operatorname{diam}(\mathbb{A}) \tag{22}$$

for all compact sets $\mathbb{A}$ *and all* $M \in \mathbb{N}$.

Note that Assumption 5.1 is automatically satisfied if standard tools from interval arithmetics are applied to bound the state trajectory $y(t,a)$ since the function $y(t,\cdot)$ is Lipschitz continuous. On the other hand, Assumption 5.2 requires that the bounds on the image set $\mathbb{E}_M(t,a)$ inherit the exponential convergence property established in Theorem 4.1. In particular, this assumption is satisfied by applying the bounding procedure described in Appendix B.

In order to simplify the convergence argumentation, the case without state constraints, i.e., $\mathbb{F}_x(t) = \mathbb{R}^{n_x}$, is addressed first.

Lemma 5.1 *Let Assumptions* 5.1 *and* 5.2 *and blanket Assumptions* A1, A2, *and* A4 *be satisfied, and suppose that* $\mathbb{F}_x(t) = \mathbb{R}^{n_x}$. *Then, for any finite tolerance* $\varepsilon > 0$, *Algorithm* 3 *applies at most*

$$\overline{M} = \left\lceil \frac{1}{C_{\mathbb{E}}^1}\left(\log\left(\frac{L_\Psi(1+\varrho)}{\varepsilon}\right) + C_{\mathbb{E}}^0\right)\right\rceil \tag{23}$$

lifting steps, where $L_\Psi < \infty$ *stands for the Lipschitz constant of the Mayer term* Ψ.

Proof Let $\mathbb{A}$ be any compact set. Since $\mathbb{F}_x(t) \ominus \overline{\mathbb{E}}_M(t,\mathbb{A}) = \mathbb{R}^{n_x}$, we have either $\overline{U}_M(\mathbb{A}) = \underline{L}_M(\mathbb{A}) = \infty$ or

$$\overline{U}_M(\mathbb{A}) - \underline{L}_M(\mathbb{A}) \le L_\Psi \operatorname{diam}\bigl(\overline{\mathbb{Y}}(T,\mathbb{A}) \oplus \overline{\mathbb{E}}_M(T,\mathbb{A})\bigr). \tag{24}$$

The former can only occur if $\mathbb{A} \cap \mathbb{D}_{\overline{M}} = \varnothing$, in which case the set $\mathbb{A}$ would be fathomed by Algorithm 3. Therefore, a lifting is only applied if

$$\begin{aligned}\overline{U}_M(\mathbb{A}) - \underline{L}_M(\mathbb{A}) &\le L_\Psi(1+\varrho)\max_{A\in\mathcal{A}} \operatorname{diam}\bigl(\overline{\mathbb{E}}_M\bigl(T,\{\operatorname{mid}(\mathbb{A})\}\bigr)\bigr)\\ &\le L_\Psi(1+\varrho)\exp\bigl(C_{\mathbb{E}}^0 - C_{\mathbb{E}}^1 M\bigr),\end{aligned}$$

which follows by substituting the lifting condition (19) in (24). Since $L_\Psi(1+\varrho)\times\exp(C^0_{\mathbb{E}}-C^1_{\mathbb{E}}M)$ can be made as close to zero as desired by increasing M and is independent of $\mathbb{A}$, there exists $\overline{M}<\infty$ such that

$$\overline{U}_{\overline{M}}(\mathbb{A})-\underline{L}_{\overline{M}}(\mathbb{A})\le\varepsilon$$

for every compact set $\mathbb{A}$ with $\mathbb{A}\cap\mathbb{D}_{\overline{M}}\neq\varnothing$. In particular, (23) yields an upper bound on the number of lifting steps applied by Algorithm 3. □

Observe that Lemma 5.1 provides an upper bound on the number of lifting operations applied by Algorithm 3 for a given tolerance $\varepsilon>0$, but it does not establish finite termination of Algorithm 3. This result is established in the following theorem under the additional assumption that the branching operation is exhaustive for every given parameterization order M.

Theorem 5.1 *Let Assumptions 5.1 and 5.2 and blanket Assumptions* A1, A2, *and* A4 *be satisfied, and suppose that $\mathbb{F}_x(t)=\mathbb{R}^{n_x}$. If the branching operation is exhaustive for every given parameterization order $M\in\mathbb{N}$, then Algorithm 3 terminates finitely for any finite tolerance $\varepsilon>0$ and any lifting parameter $\varrho>0$.*

Proof By contradiction, assume that Algorithm 3 does not terminate finitely. From Lemma 5.1, the maximum number M^* of lifting operations applied by Algorithm 3 is such that $M^*\le\overline{M}$, that is, M^* is attained after a finite number of branching operations, and the algorithm then keeps branching forever, so that the following conditions remain satisfied for an infinite number of iterations:

$$\mathcal{A}\neq\varnothing\quad\text{and}\quad\varepsilon<\min_{\mathbb{A}\in\mathcal{A}}\overline{U}_{M^*}(\mathbb{A})-\min_{\mathbb{A}\in\mathcal{A}}\underline{L}_{M^*}(\mathbb{A}).$$

By Assumptions 5.1 and 5.2 it follows that

$$\begin{aligned}\varepsilon&\overset{(24)}{<}L_\Psi\max_{\mathbb{A}\in\mathcal{A}}\operatorname{diam}\bigl(\overline{\mathbb{Y}}(T,\mathbb{A})\oplus\overline{\mathbb{E}}_{M^*}(T,\mathbb{A})\bigr)\\&\le\max_{\mathbb{A}\in\mathcal{A}}L_\Psi\bigl(C_Y+C^2_{\mathbb{E}}\bigr)\operatorname{diam}(\mathbb{A})+L_\Psi\max_{\mathbb{A}\in\mathcal{A}}\operatorname{diam}\bigl(\overline{\mathbb{E}}_{M^*}\bigl(T,\{\operatorname{mid}(\mathbb{A})\}\bigr)\bigr)\\&\le\max_{\mathbb{A}\in\mathcal{A}}L_\Psi\bigl(C_Y+C^2_{\mathbb{E}}\bigr)\operatorname{diam}(\mathbb{A})+L_\Psi\exp\bigl(C^0_{\mathbb{E}}-C^1_{\mathbb{E}}M^*\bigr).\end{aligned}$$

Since the branching operation is exhaustive for any parameterization order M, in particular M^*, we have that $\operatorname{diam}(\mathbb{A})=0$ in the limit, and therefore,

$$\varepsilon\le L_\Psi\exp\bigl(C^0_{\mathbb{E}}-C^1_{\mathbb{E}}M^*\bigr)\le L_\Psi\exp\bigl(C^0_{\mathbb{E}}-C^1_{\mathbb{E}}\overline{M}\bigr)\overset{(23)}{\le}\frac{\varepsilon}{1+\varrho}.$$

Finally, since the inequality $\varepsilon\le\frac{\varepsilon}{1+\varrho}$ cannot be satisfied for both $\varepsilon>0$ and $\varrho>0$, we obtain a contradiction. □

While Theorem 5.1 is based solely on assumptions that are verifiable a priori, the situation becomes more involved as soon as general state constraints are present. This is because the upper-bounding problem can fail to determine a finite upper bound within a finite number of branch-and-lift iterations with such constraints. Nonetheless, this problem is not specific to the proposed branch-and-lift algorithm, but it is a known problem of branch-and-bound in general, as discussed in [59–61].

In the following two subsections, we analyze the finite convergence of Algorithm 3 in the presence of state constraints under the additional condition that either a particular constraint qualification holds, or a reliable (local) optimal control solver is available.

5.4.1 Finite Termination with General State Constraints via a Constraint Qualification

A guarantee of finite termination with Algorithm 3 in the presence of general state constraints can be obtained by enforcing a certain constraint qualification. The following assumption is similar in essence to the constraint qualification imposed by Bhattacharjee et al. [65] in the context of semi-infinite programming.

Assumption 5.3 *The optimal control problem* (1) *is strictly feasible in the sense that there exists a sequence of feasible L^2-integrable functions $\{u_i\}_{i\in\mathbb{N}}$ such that*

$$\forall (t,i) \in [0,T] \times \mathbb{N}, \quad u_i(t) \in \mathbb{F}_u(t), \quad x(t,u_i) \in \operatorname{int}\bigl(\mathbb{F}_x(t)\bigr), \quad \textit{and}$$
$$\lim_{i\to\infty} \max_{t\in[0,T]} \bigl\| u_i(t) - u^*(t) \bigr\| = 0$$

for at least one global minimizer u^* of (1), *where* $\operatorname{int}(\mathbb{F}_x(t))$ *denotes the interior of the set $\mathbb{F}_x(t)$.*

It is important to note that such a constraint qualification fails to hold for many optimal control problems in practice. In the case of optimal control problems with terminal equality constraints, for instance, one has $\operatorname{int}(\mathbb{F}_x(T)) = \varnothing$. Nonetheless, the following finite-termination result can be established under this assumption.

Corollary 5.1 *Let Assumptions* 5.1, 5.2, *and* 5.3 *and blanket Assumptions* A1, A2, A3, *and* A4 *be satisfied. If the branching operation is exhaustive for every given parameterization order $M \in \mathbb{N}$, then Algorithm* 3 *terminates finitely.*

Proof Assumption 5.3 implies that there exists a feasible ε-suboptimal solution $u_\varepsilon^* \in L^2[0,T]^{n_u}$ of (1) satisfying $x(t,u_\varepsilon^*) \in \operatorname{int}(\mathbb{F}_x(t))$ for all $t \in [0,T]$. Since $\operatorname{diam}(\overline{\mathbb{E}}_M(t,\mathbb{A}))$ converges to zero for $M \to \infty$ and $\operatorname{diam}(\mathbb{A}) \to 0$ (Assumption 5.2), it follows that for all sufficiently large $M < \infty$ and all sufficiently small $\delta > 0$, we have

$$\underline{\mathbb{Y}}(t,\mathbb{A}) \subseteq \mathbb{F}_x(t) \ominus \overline{\mathbb{E}}_M(t,\mathbb{A})$$

for all compact sets $\mathbb{A}$ satisfying $\operatorname{diam}(\mathbb{A}) \le \delta$ and

$$\left(\frac{1}{\sigma_0} \langle u_\varepsilon^*, \Phi_0 \rangle_\mu^\mathsf{T}, \ldots, \frac{1}{\sigma_M} \langle u_\varepsilon^*, \Phi_M \rangle_\mu^\mathsf{T} \right)^\mathsf{T} \in \mathbb{A}.$$

Consequently, $U_M(\mathbb{A}) < \infty$ for all sufficiently small sets $\mathbb{A}$ contained in a small neighborhood of the Gram–Schmidt projection of u_ε^*, thereby allowing us to transfer the proofs of Lemma 5.1 and Theorem 5.1 line-by-line to arrive at the result. □

5.4.2 Finite Termination with General State Constraints based on a Reliable Local Optimal Control Solver

An alternative way of obtaining a guarantee of finite termination with Algorithm 3, which removes the need for the constraint qualification in Assumption 5.3, is by assuming that a reliable local optimal control solver is available.

Definition 5.1 An optimal control solver is said to be *locally reliable* for the problem (1) under a given control parameterization $\{\Phi_i\}_{i\in\mathbb{N}}$ if, for all $M \in \mathbb{N}$, there exists $\delta > 0$ such that this solver returns a feasible solution of problem (13) for all compact sets $\mathbb{A}$ with $\mathrm{diam}(\mathbb{A}) \le \delta$ and $\mathcal{V}_M^*(\mathbb{A}) < \infty$.

Unfortunately, currently available implementations of local optimal control solver do not come along with such local reliability guarantees and may fail to find feasible solutions for certain degenerate state constraint geometries, such as optimal control problems having a single feasible point. In the authors' experience, however, local optimal control solvers work well for practical and well-formulated optimal control problems, especially when initialized near a locally optimal solution. The following finite-termination result holds under the assumption that a reliable local optimal control solver is available.

Corollary 5.2 *Let the optimal control problem* (1) *be feasible, and suppose that a reliable local optimal control solver is available. For any compact set* $\mathbb{A} \in \mathcal{A}$ *with* $\mathrm{diam}(\mathbb{A}) \le \delta$ *and* $\mathcal{V}_M^*(\mathbb{A}) < \infty$, *let the inner-approximation function* $\underline{\mathbb{Y}}(\cdot, \mathbb{A})$ *be obtained as*

$$\forall t \in [0, T] \quad \underline{\mathbb{Y}}(t, \mathbb{A}) := \left\{ y\left(t, \left(\frac{1}{\sigma_0}\langle \bar{u}, \Phi_0\rangle_\mu^\mathsf{T}, \ldots, \frac{1}{\sigma_M}\langle \bar{u}, \Phi_M\rangle_\mu^\mathsf{T}\right)^\mathsf{T}\right)\right\},$$

where $\bar{u}$ *is a feasible solution of* (13). *Let also Assumptions* 5.1 *and* 5.2 *and blanket Assumptions* A1, A2, A3, *and* A4 *be satisfied. If the branching operation is exhaustive for every given parameterization order* $M \in \mathbb{N}$, *then Algorithm* 3 *terminates finitely.*

Proof The proof of this statement is analogous to the proof of Theorem 5.1 with the only difference that the convergence of the upper bound is now guaranteed by the assumption of a reliable local optimal control solver. □

As already mentioned, neither Corollary 5.1 nor Corollary 5.2 is entirely satisfactory in that they rely on rather strong assumptions, which are not always satisfied in practice and are difficult to check a priori. We reiterate that similar problems can arise for finite-dimensional NLP problems too if suitable constraint qualifications fail to hold or if a reliable local solver is unavailable [59–61]. As such, the development of optimal control solvers that would come along with local reliability guarantees under preferably mild constraint qualifications remains an important topic for future research.

Finally, we consider the more general case that the functions f and G in (1) are locally, but not globally, Lipschitz continuous, that is, the solution trajectories $x(t,u)$ and $y(t,a)$ may not exist on all of $[0,T]$ for certain choices of u and a due to the presence of a finite escape time. We start by noting that state-of-the-art enclosure methods for nonlinear ODEs can validate existence and uniqueness of the solutions [66], thereby potentially providing a mechanism to fathom control regions in which the ODEs have no solutions. But regardless, a formal proof of convergence of the branch-and-lift algorithm can still be obtained under the weaker assumptions that f and G are smooth, yet not necessarily globally Lipschitz continuous. Consider the following assumption:

A2': The functions $f:\mathbb{R}^{n_x}\to\mathbb{R}^{n_x}$ and $G:\mathbb{R}^{n_x}\to\mathbb{R}^{n_x\times n_u}$ are smooth, and there exist $\delta>0$ and a global minimizer u^* of the optimal control problem (1) such that the differential equation (9) admits a solution $x(t,u)$ for all $u\in L^2[0,T]^{n_u}$ with $\int_0^T \|u(t)-u(t^*)\|^2\,\mathrm{d}t\le\delta$.

Then, the results in Theorem 5.1 and Corollaries 5.1 and 5.2 still hold upon relaxing the blanket Assumption A2 with A2' and modifying Assumptions 5.1 and 5.2 so that (20)–(22) hold in a local neighborhood of u^*. This extension is a direct consequence of the fact that, under Assumption A2', the solution trajectories $x(\cdot,u)$ and $y(\cdot,a)$, and in turn the enclosure functions $\overline{\mathbb{Y}}(\cdot,\mathbb{A})$ and $\overline{\mathbb{E}}_M(\cdot,\mathbb{A})$, are guaranteed to exist for sufficiently large parameterization orders M in a neighborhood of u^*.

6 Numerical Case Study: Optimal Control of a Bioreactor

Rather than providing a detailed numerical implementation or performance assessment of the branch-and-lift algorithm, this section aims at demonstrating its application on a practical case study. Our implementation of Algorithm 3 is based on the ACADO Toolkit [26] as the local optimal control solver—see Sect. 5.4.2—and uses the library MC++ [58] to compute the required nonlinearity bounds and the ODE enclosures based on Taylor models combined with rigorous remainder estimates [49]. Note that this is a prototype implementation and we do not report CPU times for this reason.

The fermentation control problem considered in this case study is based on a process model that has been developed in [67, 68]. The dynamics are highly nonlinear, and several operational strategies have been reported in the literature [68–70]. To the authors' best knowledge, however, the application of a generic deterministic global optimization algorithm to find ε-suboptimal solutions has never been attempted for this problem.

Problem Definition Consider a continuous culture fermentation process described by the following dynamic model [67–69]:

$$f(x)=\begin{pmatrix} -\frac{1}{T}Dx_4 \\ -Dx_2+\mu(x_3,x_4)x_2 \\ -Dx_3-\frac{\mu(x_3,x_4)x_2}{Y_{X/S}} \\ -Dx_4+(\alpha\mu(x_3,x_4)+\beta)x_2 \\ 0 \end{pmatrix} \quad \text{and} \quad G(x)=\begin{pmatrix} 0 \\ 0 \\ D \\ 0 \\ \frac{1}{T} \end{pmatrix}$$

with

$$\mu(x_3,x_4)=\mu_{\mathrm{m}}\frac{(1-\frac{x_4}{P_{\mathrm{m}}})x_3}{K_{\mathrm{m}}+x_3+\frac{x_3^2}{K_{\mathrm{i}}}}$$

and the initial value

$$x(0)=(0,X_0,S_0,P_0,0)^{\mathsf{T}}.$$

The Mayer term in this problem is $\Psi(x)=x_1$, and the set of feasible states is given by

$$\forall t\in[0,T),\quad \mathbb{F}_x(t)=\mathbb{R}^5,\quad \text{and}\quad \mathbb{F}_x(T)=\left\{x\in\mathbb{R}^5 \;\middle|\; \begin{array}{l} x_2=X_0 \\ x_3=S_0 \\ x_4=P_0 \\ x_5=\overline{S}_{\mathrm{f}} \end{array}\right\}.$$

Moreover, the feasible control set is

$$\forall t\in[0,T],\quad \mathbb{F}_u(t):=\left\{u \mid S_{\mathrm{f}}^{\min}\le u\le S_{\mathrm{f}}^{\max}\right\},$$

and an isoperimetric constraint on the control input is defined such that

$$a_0=\int_0^T u(t)\,\mathrm{d}t=\overline{S}_{\mathrm{f}}$$

(where a_0 is the first coefficient in a control parameterization based on Legendre polynomials.) All of the model parameters are reported in Table 1.

Optimal Control Solution Figure 3 displays the optimal control and response for an ε-optimal solution, as determined by the proposed branch-and-lift algorithm with optimality tolerance $\varepsilon=0.001$ gh^{-1}L^{-1}. We find that this solution is identical to the one found in [70] by using local search methods, with some good insight on how to initialize the search. A major difference here is that the branch-and-lift algorithm comes along with a certificate that the computed solution is within 0.001 gh^{-1}L^{-1} of the actual global solution.

Discussion The focus of the ensuing discussion is on the performance of the branch-and-lift algorithm (Algorithm 3). The control parameterization at the start of the algorithm being rather coarse, we find that two lifting operations are applied during the first two branch-and-lift iterations, that is, the lifting condition (19) happens to be satisfied for $M=0$ and $M=1$ without branching. As the parameterization order is

Table 1 Fermentation process parameters

Description	Symbol	Value
Dilution rate	D	$0.15\ \mathrm{h}^{-1}$
Substrate inhibition constant	K_i	$22\ \mathrm{g\,L}^{-1}$
Substrate saturation constant	K_m	$1.2\ \mathrm{g\,L}^{-1}$
Product saturation constant	P_m	$50\ \mathrm{g\,L}^{-1}$
Yield of the biomass	$Y_{X/S}$	0.4
First product yield constant	α	2.2
Second product yield constant	β	$0.2\ \mathrm{h}^{-1}$
Specific growth rate scale	μ_m	$0.48\ \mathrm{h}^{-1}$
Average feed substrate concentration	$\overline{S}_\mathrm{f}$	$32.0\ \mathrm{g\,L}^{-1}$
Minimum feed substrate concentration	$S_\mathrm{f}^\mathrm{min}$	$28.0\ \mathrm{g\,L}^{-1}$
Maximum feed substrate concentration	$S_\mathrm{f}^\mathrm{max}$	$40.0\ \mathrm{g\,L}^{-1}$
Duration of one period	T	48 h
Biomass initial condition	X_0	$6.9521\ \mathrm{g\,L}^{-1}$
Substrate initial condition	S_0	$13.4166\ \mathrm{g\,L}^{-1}$
Product initial condition	P_0	$24.1566\ \mathrm{g\,L}^{-1}$

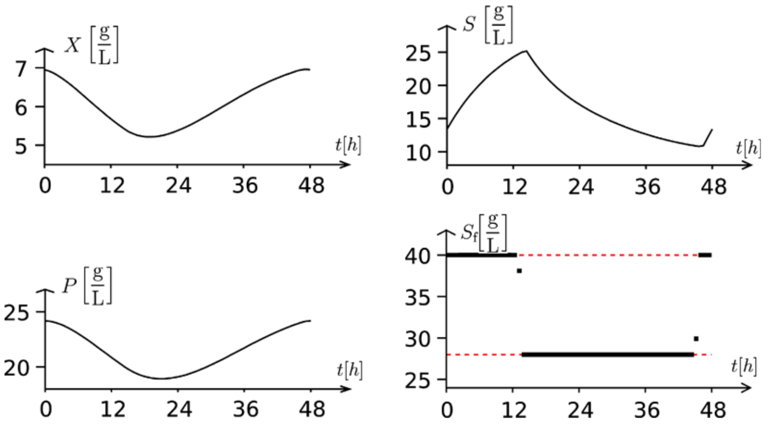

Fig. 3 The state trajectories "$X = x_2$", "$S = x_3$", and "$P = x_4$" as well as the control trajectory "$S_\mathrm{f} = u$" corresponding to an ε-optimal solution of the fermentation process case study, with accuracy $\varepsilon = 0.001\ \mathrm{g\,h^{-1}\,L^{-1}}$

increased to $M = 2$, however, the algorithm performs a number of branching operations and the fathoming test successfully excludes a number of suboptimal control regions. The projection onto the (a_1, a_2)-plane of the partition $\mathcal{A}$ at the order $M = 2$ is shown as the grey-shaded area on the left plot in Fig. 4—recall that $a_0 = \overline{S}_\mathrm{f}$ due to the isoperimetric constraint. The intervals $[\underline{a}_1, \overline{a}_1]$ and $[\underline{a}_2, \overline{a}_2]$ reported on this plot are those computed during the first and second lifting steps, and the unshaded part of the box $[\underline{a}_1, \overline{a}_1] \times [\underline{a}_2, \overline{a}_2]$ shows the control subregion that is excluded before the third lifting step—i.e., from $M = 2$ to $M = 3$—is applied. Represented on the right plot in Fig. 4 are the projections onto the (a_1, a_2)-plane of the partition $\mathcal{A}$ before the third,

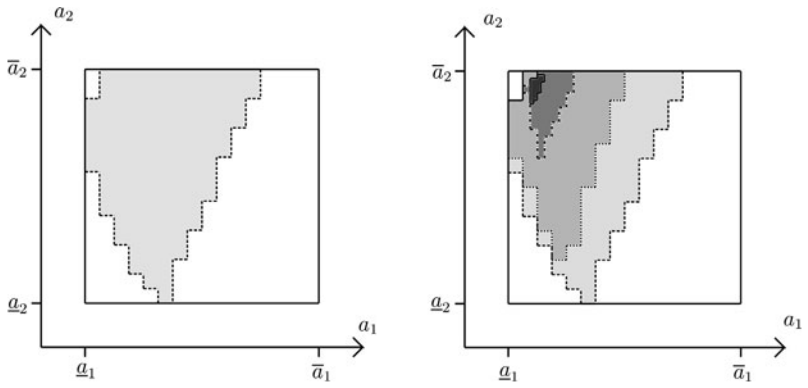

Fig. 4 *Left plot*: projection of the partition $\mathcal{A}$ onto the (a_1, a_2)-plane (*grey shaded area*) before the third lifting step is performed. *Right plot*: Projection of the partition $\mathcal{A}$ onto the (a_1, a_2)-plane before the third, fourth, fifth, and sixth lifting steps, i.e., for $M \in \{2, 3, 4, 5\}$

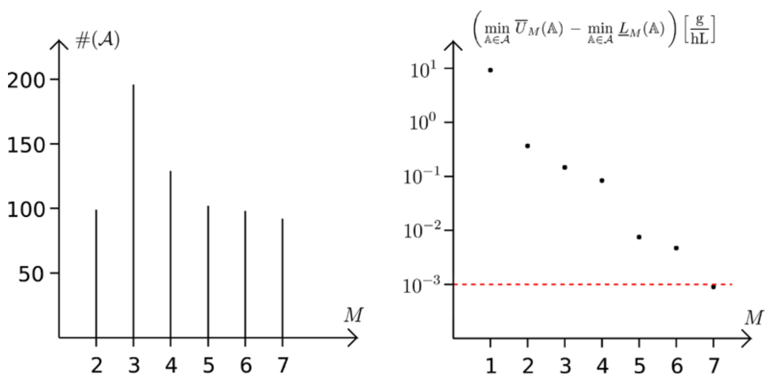

Fig. 5 *Left*: The number of boxes in the set family $\mathcal{A}$ for $M = 2, \ldots, 7$ before applying the next lifting step. *Right*: The gap between upper and lower bound for $M = 1, 2, \ldots, 7$

fourth, fifth, and sixth lifting steps, with darker grey shades corresponding to more refined control parameterizations. Observe, in particular, how the region in which the globally optimal control coefficients a_1 and a_2 belong progressively shrinks as the control parameterization is refined.

The left plot in Fig. 5 displays the cardinality of the partition $\mathcal{A}$ immediately before the next lifting operation is applied, here for parameterization orders $M = 2, \ldots, 7$. Note that the partition size remains rather small, between 100–200 subsets, and it even decreases for larger M. The right part of Fig. 5 shows the decrease in the optimality gap $(\min_{\mathbb{A}\in\mathcal{A}} \overline{U}_M(\mathbb{A}) - \min_{\mathbb{A}\in\mathcal{A}} \underline{L}_M(\mathbb{A}))$ between the upper and lower bounds on the optimal value $\mathcal{V}$ as the parameterization order M is increased, until the desired tolerance ε is attained.

In this case study, Algorithm 3 stops after 810 iterations, taking approximately 2.5 hours to converge and finding the solution that is displayed in Fig. 3.

7 Conclusions

This paper has presented a new branch-and-lift algorithm for solving nonlinear optimal control problems with smooth nonlinear dynamics and nonconvex objective and constraints to guaranteed global optimality. Particular emphasis has been on the convergence properties of the image of the control parameterization error in state space, which are summarized in Theorem 4.1. Another principal contribution of this paper has been the introduction of a lifting operation in Sect. 5, which adapts the control parameterization accuracy during the global search. The most important result of this paper is that the proposed branch-and-lift algorithm can find ε-suboptimal solutions of the continuous-time optimal control problem (1) in a finite number of iterations, as proven in Theorem 5.1 and Corollaries 5.1 and 5.2. As far as the authors are aware, this algorithm is the first complete search method of its kind, apart from algorithms based on dynamic programming. Finally, the performance of the proposed branch-and-lift algorithm has been illustrated for the optimal control of a periodic fermentation process.

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Appendix A: Proof of Theorem 4.1

This section aims at constructing convergent bounds on the set $\mathbb{E}_M(t,a)$, thereby providing a proof of Theorem 4.1. Recall the definition of the set $\mathbb{E}_M(t,a)$ in Sect. 4 as

$$\mathbb{E}_M(t,a) := \left\{ x(t,u) - y(t,a) \mid u \in \mathbb{U}_M(a) \right\}.$$

The blanket Assumption A2 guarantees that the solution trajectories x and y are well defined, so that a sufficiently large and compact a priori enclosure $\widetilde{\mathbb{E}} \subseteq \mathbb{R}^{n_x}$ can always be found such that

$$\forall t \in [0,T], \quad \mathbb{E}_M(t,a) \subseteq \widetilde{\mathbb{E}}.$$

The focus here is on tightening the a priori enclosure $\widetilde{\mathbb{E}}$, which is crucial for analyzing the convergence of the set $\mathbb{E}_M(t,a)$. We start by defining the response defect

$$d(t,u,a) = x(t,u) - y(t,a),$$

which by construction satisfies an ODE of the form

$$\begin{aligned} &\forall t \in [0,T], \\ &\dot{d}(t,u,a) \overset{(3,9)}{=} f\big(x(t,u)\big) - f\big(y(t,a)\big) + G\big(x(t,u)\big)u(t) - G\big(y(t,a)\big)\left(\sum_{i=0}^{M} a_i \Phi_i(t)\right) \\ &\text{with} \quad d(0,u,a) = 0. \end{aligned} \tag{25}$$

In order to bound the solution trajectory of (25), consider a Taylor expansion of the term $f(x(t,u)) - f(y(t,a))$ in the form

$$f\big(x(t,u)\big) - f\big(y(t,a)\big) = \frac{\partial f(y(t,a))}{\partial x} d(t,u,a) + R_f(t,u,a) d(t,u,a),$$

where the matrix $R_f(t,u,a) \in \mathbb{R}^{n_x \times n_x}$ denotes a nonlinear remainder term. By the mean-value theorem, R_f is bounded as

$$\forall u \in \mathbb{U}_M(a), \quad \big\| R_f(t,u,a) \big\| \le \max_{d',d'' \in \widetilde{\mathbb{E}}} \left\| \frac{1}{2} \frac{\partial^2 f(y(t,a)+d')}{\partial x^2} d'' \right\|. \tag{26}$$

Similarly, the mean-value theorem can be applied to the term $[G(x(t,u)) - G(y(t,a))]u(t)$, giving

$$\big[G\big(x(t,u)\big) - G\big(y(t,a)\big)\big]u(t) = R_G(t,u,a) d(t,u,a),$$

where the nonlinear remainder term $R_G(t,u,a)$ is bounded by

$$\forall u \in \mathbb{U}_M(a), \quad \big\| R_G(t,u,a) \big\| \le \max_{u' \in \mathbb{F}_u(t)} \max_{d' \in \widetilde{\mathbb{E}}} \left\| \frac{\partial G(y(t,a)+d')}{\partial x} u' \right\|. \tag{27}$$

In the following, we introduce the shorthand notation $R(t,u,a) := R_f(t,u,a) + R_G(t,u,a)$, so that (25) can be written in the form

$$\begin{aligned} &\forall t \in [0,T], \\ &\dot{d}(t,u,a) = \frac{\partial f(y(t,a))}{\partial x} d(t,u,a) + R(t,u,a) d(t,u,a) \\ &\qquad + G\big(y(t,a)\big)\left[u(t) - \sum_{i=0}^{M} a_i \Phi_i(t) \right] \quad \text{with } d(0,u,a) = 0. \end{aligned} \tag{28}$$

A few remarks are in order regarding the previous ODE (28):

1. The Jacobian of f and the function G are evaluated at the point $y(t,a)$. Therefore, these matrices are independent of the control input u.
2. The matrix-valued remainder term $R(t,u,a)$ depends on u in general, but standard tools such as interval arithmetics can be applied to construct a bound $\overline{R}(t,a) < \infty$ independent of u such that

$$\begin{aligned} &\forall t \in [0,T], \\ &\max_{d',d'' \in \widetilde{\mathbb{E}}} \left\| \frac{\partial^2 f(y(t,a)+d')}{\partial x^2} \frac{d''}{2} \right\|_2 + \max_{u' \in \mathbb{F}_u(t)} \max_{d' \in \widetilde{\mathbb{E}}} \left\| \frac{\partial G(y(t,a)+d')}{\partial x} u' \right\|_2 \le \overline{R}(t,a). \end{aligned} \tag{29}$$

   The validity of this bound follows from the inequalities (26) and (27):

$$\forall u \in \mathbb{U}_M(a), \quad \big\| R(t,u,a) \big\|_2 \le \overline{R}(t,a).$$

However, the tightness of the bound $\overline{R}(t,a)$ depends strongly on the tightness of the a priori enclosure $\widetilde{\mathbb{E}}$, and a tighter $\widetilde{\mathbb{E}}$ will typically lead to a tighter bound on the norm of the remainder term R.

3. The right-hand side of the ODE (28) also depends on the control parameterization defect $(u - \sum_{i=0}^{M} a_i \Phi_i)$. It follows by the orthogonality of the Φ_is that the first $M+1$ Gram–Schmidt coefficients of this defect are all equal to zero. Consequently, an enclosure $\mathbb{W}_M(a)$ of the control parameterization defect, which is independent of u and convex (Assumption A4), is obtained as:

$$\forall u \in \mathbb{U}_M(a),$$
$$u - \sum_{i=0}^{M} a_i \Phi_i \in \mathbb{W}_M(a) := \left\{ w \in L^2[0,T]^{n_u} \;\middle|\; \begin{array}{l} \forall i \in \{0,\ldots,M\}, \forall t \in [0,t], \\ 0 = \langle w, \Phi_i \rangle_\mu \\ w(t) + \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t) \end{array} \right\}. \tag{30}$$

Summarizing the above considerations, the main idea is to regard the solution trajectory of the differential equation (28) as a function of the remainder term and of the control parameterization defect rather than as a function of the control function u. In order to formalize this change of variable, let $e(t,\Delta,w)$ denote the solution of the ODE

$$\dot{e}(t,\Delta,w) = \big[A(t) + \Delta(t)\big] e(t,\Delta,w) + B(t) w(t), \quad \text{with } e(0,\Delta,w) = 0, \tag{31}$$

for any functions $w \in L^2[0,T]^{n_u}$ and $\Delta \in L^2[0,T]^{n_x \times n_x}$, where we have introduced the shorthand notations $A(t) := \frac{\partial f(y(t,a))}{\partial x}$ and $B(t) := G(y(t,a))$.

Proposition A.1 *Let $\overline{R}(\cdot,a)$ be a remainder bound satisfying* (29), *and let $\mathbb{W}_M(a)$ be defined by* (30). *Then,*

$$\forall (t,a) \in [0,T] \times \mathbb{D}_M,$$
$$\mathbb{E}_M(t,a) \subseteq \left\{ e(t,\Delta,w) \;\middle|\; \begin{array}{l} w \in \mathbb{W}_M(a) \\ \forall \tau \in [0,T] \quad \|\Delta(\tau)\|_2 \le \overline{R}(\tau,a) \end{array} \right\},$$

where $e(\cdot,\Delta,w)$ denotes the solution of (31).

Proof From the definition of the defect function d we have

$$\mathbb{E}_M(t,a) = \big\{ d(t,u,a) \mid u \in \mathbb{U}_M(a) \big\}.$$

Moreover, the function e is defined such that

$$d(t,u,a) = e\left(t, R(\cdot,u,a), u - \sum_{i=0}^{M} a_i \Phi_i \right).$$

Therefore, the result of the proposition follows by applying the change of variables

$$R(\cdot, u, a) \to \Delta \quad \text{and} \quad u - \sum_{i=0}^{M} a_i \Phi_i \to w$$

and using that $\overline{R}(\cdot, a)$ and $\mathbb{W}_M(a)$ are bounds on the norm of the remainder term and on the control parameterization defect, respectively. $\square$

In order to understand the motivation behind Proposition A.1, it is helpful to interpret the differential equation (31) as a low-pass filter with uncertain but bounded gain Δ, which would filter high-frequency modes of the "noise" w. This interpretation is useful, as the control parameterization defect $w = u - \sum_{i=0}^{M} a_i \Phi_i$ is bounded by the set $W_M(a)$. For example, if $\Phi_0, \Phi_1, \ldots$ denote the basis functions in a standard trigonometric Fourier expansion, the set $\mathbb{W}_M(a)$ contains for large M only highly oscillatory functions, as the first $M+1$ Fourier coefficients of the control parameterization are zero in this case. The differential equation (31) can be expected to filter out these highly oscillating modes such that $e(t, \Delta, w) \approx 0$. Having this interpretation in mind, intuition suggests that we should be able to compute tight bounds on the function $e(t, \Delta, w)$, which converge for $M \to \infty$, even when the uncertain gain Δ is not known exactly.

The aim of the following considerations is to formalize this intuition by translating it into a rigorous algorithm that computes convergent enclosures of the sets $\mathbb{E}_M(\cdot, a)$ on $[0, T]$. To do so, the function $e(t, \Delta, w)$ is decomposed into the sum of two functions $e_{\mathrm{L}}(t, w)$ and $e_{\mathrm{N}}(t, \Delta, v)$ such that

$$e(t, \Delta, w) = e_{\mathrm{L}}(t, w) + e_{\mathrm{N}}\big(t, \Delta, e_{\mathrm{L}}(\cdot, w)\big).$$

Specifically, $e_{\mathrm{L}}(\cdot, w)$ and $e_{\mathrm{N}}(\cdot, \Delta, v)$ are the solutions of the following auxiliary ODEs:

$$\forall t \in [0, T],$$

$$\dot{e}_{\mathrm{L}}(t, w) = A(t) e_{\mathrm{L}}(t, w) + B(t) w(t) \quad \text{with} \;\; e_{\mathrm{L}}(0, w) = 0, \tag{32}$$

$$\dot{e}_{\mathrm{N}}(t, \Delta, v) = \big(A(t) + \Delta(t)\big) e_{\mathrm{N}}(t, \Delta, v) + \Delta(t) v(t) \quad \text{with} \;\; e_{\mathrm{N}}(t, \Delta, v) = 0. \tag{33}$$

Note that the output e_{L} of the first ODE (32) becomes an input in the second ODE (33). Moreover, we define the sets

$$\mathbb{E}_M^{\mathrm{L}}(t, a) := \big\{ e_{\mathrm{L}}(t, w) \mid w \in \mathbb{W}_M(a) \big\} \quad \text{and}$$

$$\mathbb{E}_M^{\mathrm{N}}(t, a) := \left\{ e_{\mathrm{N}}(t, \Delta, v) \;\middle|\; \forall \tau \in [0, t], \quad \begin{array}{l} v(\tau) \in \mathbb{E}_M^{\mathrm{L}}(\tau, a) \\ \|\Delta(\tau)\|_2 \leq \overline{R}(\tau, a) \end{array} \right\}.$$

The following proposition is a direct consequence of Proposition A.1 and of the foregoing decomposition.

Proposition A.2 *The image set $\mathbb{E}_M(t,a)$ is contained in the Minkowski sum of the sets $\mathbb{E}_M^{\mathrm{L}}(t,a)$ and $\mathbb{E}_M^{\mathrm{N}}(t,a)$,*

$$\forall (t,a) \in [0,T] \times \mathbb{D}_M, \quad \mathbb{E}_M(t,a) \subseteq \mathbb{E}_M^{\mathrm{L}}(t,a) \oplus \mathbb{E}_M^{\mathrm{N}}(t,a). \tag{34}$$

The following lemma establishes that, in order to find a convergent bound on the diameter of the set $\mathbb{E}_M(t,a)$, it is sufficient to find a convergent bound on the diameter of the set $\mathbb{E}_M^{\mathrm{L}}(t,a)$.

Lemma A.1 *There exists a constant $\ell(t) < \infty$ such that*

$$\forall t \in [0,T], \quad \operatorname{diam}\big(\mathbb{E}_M(t,a)\big) \le \ell(t) \max_{\tau \in [0,T]} \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{L}}(\tau,a)\big).$$

Proof Since the uncertain gain Δ is bounded, there exist constants ℓ_1 and ℓ_2 such that

$$\big\| A(t) + \Delta(t) \big\|_2 \le \ell_1 \quad \text{and} \quad \big\| \Delta(t) v(t) \big\|_2 \le \ell_2 \frac{\operatorname{diam}(\mathbb{E}_M^{\mathrm{L}}(t,a))}{2}$$

for all v with $v(t) \in \mathbb{E}_M^{\mathrm{L}}(t,a)$, all Δ with $\|\Delta(t)\|_2 \le \overline{R}(t,a)$, and all $t \in [0,T]$. Applying Gronwall's lemma for bounding the norm of the solution of the differential equation (33) yields the following bound on the diameter of $\mathbb{E}_M^{\mathrm{N}}(t,a)$:

$$\operatorname{diam}\big(\mathbb{E}_M^{\mathrm{N}}(t,a)\big) \le \exp(\ell_1 t)\ell_2 \max_{\tau \in [0,T]} \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{L}}(\tau,a)\big).$$

Then from Proposition A.2 it follows that

$$\begin{aligned} \operatorname{diam}\big(\mathbb{E}_M(t,a)\big) &\le \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{L}}(t,a)\big) + \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{N}}(t,a)\big) \\ &\le \big[1 + \ell_2 \exp(\ell_1 t)\big] \max_{\tau \in [0,T]} \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{L}}(\tau,a)\big), \end{aligned} \tag{35}$$

and the result follows by defining $\ell(t) := 1 + \ell_2 \exp(\ell_1 t)$. □

In the remainder of this appendix, the focus is on bounding the set $\mathbb{E}_M^{\mathrm{L}}(t,a)$. We start by noting that the image sets $\mathbb{E}_M^{\mathrm{L}}(t,a)$ are both compact and convex. The compactness of $\mathbb{E}_M^{\mathrm{L}}(t,a)$ follows from Filippov's theorem [62]. Moreover, the convexity of $\mathbb{E}_M^{\mathrm{L}}(t,a)$ follows from the fact that linear transformations of convex sets are convex, recalling that the set $\mathbb{W}_M(a)$ is convex and that the functional $e_{\mathrm{L}}(t,\cdot)$ is linear since the ODE (32) is itself linear; see also [71]. Because any compact and convex set is uniquely characterized by its support function [72], we define the support function $V(t,\cdot) : \mathbb{R}^{n_x} \to \mathbb{R}$ associated with the image set $\mathbb{E}_M^{\mathrm{L}}(t,a)$ by

$$\forall c \in \mathbb{R}^{n_x}, \quad V(t,c) := \max_{w \in \mathbb{W}_M(a)} c^{\mathsf{T}} e_{\mathrm{L}}(t,w). \tag{36}$$

It is not hard to see from (36) that

$$\sup_c \frac{V(t,c)}{\|c\|_2} \ge \frac{1}{2} \operatorname{diam}\big(\mathbb{E}_M^{\mathrm{L}}(t,a)\big),$$

thereby providing a means for bounding the diameter of $\mathbb{E}_M^{\mathsf{L}}(t,a)$. In expanded form, $V(t,c)$ reads

$$V(t,c) := \max_{w \in L^2[0,T]^{n_u}} \quad c^\mathsf{T} \int_0^t Z(t,\tau) B(\tau) w(\tau)\, \mathrm{d}\tau \tag{37}$$
$$\text{s.t.} \quad \begin{cases} \forall i \in \{0,\dots,M\} \quad \forall t \in [0,t], \\ 0 = \langle w, \Phi_i \rangle_\mu, \\ w(t) + \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t), \end{cases}$$

with $Z : [0,T] \times [0,T] \to \mathbb{R}^{n_x \times n_x}$ the fundamental solution of the parametric linear ODE (32), which satisfies

$$\forall \tau, t \in [0,T], \qquad \frac{\partial}{\partial t} Z(t,\tau) = A(t) Z(t,\tau) \quad \text{with } Z(\tau,\tau) = I.$$

Since the sets $\mathbb{F}_u(t)$ are compact, one can always scale the dynamic system, and we shall therefore restrict the analysis to the L^2-integrable functions w with $w(t) + \sum_{i=0}^{M} a_i \Phi_i(t) \in \mathbb{F}_u(t)$ for all $t \in [0,T]$ and such that

$$\|w\|_{\mu,2} := \int_0^T w(t)^\mathsf{T} w(t) \mu(t)\, \mathrm{d}t \le 1.$$

Let the functions $H_t : [0,T] \to \mathbb{R}^{n_x \times n_x}$ and $\theta : [0,T] \times [0,T] \to \mathbb{R}$ be defined by

$$H_t(\tau) := \frac{1}{\mu(\tau)} Z(t,\tau) B(\tau) \theta(t,\tau) \quad \text{and} \quad \theta(t,\tau) := \begin{cases} 1 & \text{if } \tau \le t, \\ 0 & \text{otherwise}, \end{cases}$$

for all $t, \tau \in [0,T]$. The objective function in (38) can be written in the form

$$\begin{aligned} c^\mathsf{T} \int_0^t Z(t,\tau) B(\tau) w(\tau)\, \mathrm{d}\tau &= c^\mathsf{T} \int_0^T \frac{1}{\mu(\tau)} Z(t,\tau) B(\tau) \theta(t,\tau) w(\tau) \mu(\tau)\, \mathrm{d}\tau \\ &= \langle c^\mathsf{T} H_t, w \rangle_\mu, \end{aligned}$$

and an upper bound on the support function $V(t,c)$ is given by

$$V(t,c) \le \max_w \langle c^\mathsf{T} H_t, w \rangle_\mu \quad \text{s.t.} \quad \begin{cases} 0 = \langle w, \Phi_i \rangle_\mu \quad \forall i \in \{0,\dots,M\}, \\ \|w\|_{\mu,2} \le 1. \end{cases} \tag{38}$$

Associating with each equality constraint $0 = \langle w, \Phi_i \rangle_\mu$ in (38) the scaled multipliers $c^\mathsf{T} D_i \in \mathbb{R}^{n_u}$, the dual of the convex problem (38) gives

$$V(t,c) \le \inf_D \max_w \langle c^\mathsf{T} H_t, w \rangle_\mu - \sum_{i=0}^{M} c^\mathsf{T} D_i \langle \Phi_i, w \rangle_\mu \quad \text{s.t.} \quad \|w\|_{\mu,2} \le 1$$

$$= \inf_{D} \left\| c^{\mathsf{T}} \left(H_t - \sum_{i=0}^{M} D_i \Phi_i \right) \right\|_{\mu,2} = \left\| c^{\mathsf{T}} \left(H_t - \sum_{i=0}^{M} \frac{\langle H_t, \Phi_i \rangle_\mu}{\sigma_i} \Phi_i \right) \right\|_{\mu,2} \tag{39}$$

where the tight version of the Cauchy–Schwarz inequality for L_2-scalar products has been used in the last equality. At this point, it becomes clear that the derived bound on the support function $V(t,c)$ depends crucially on how accurately the function H_t can be approximated with the function $\sum_{i=0}^{M} D_i \Phi_i$. This observation is formalized in the following theorem.

Theorem A.1 *Let Assumption* 4.1 *and blanket Assumptions* A2 *and* A4 *be satisfied. Then, there exist constants* $C_E^{L,0} \in \mathbb{R}$ *and* $C_E^{L,1} \in \mathbb{R}_{++}$ *such that the condition*

$$\forall (t,a) \in [0,T] \times \mathbb{D}_M, \quad \log\big(\mathrm{diam}\big(\mathbb{E}_M^{\mathrm{L}}(t,a)\big)\big) \le C_E^{L,0} - C_E^{L,1} M$$

is satisfied for all $M \in \mathbb{N}$.

Proof Since the function H_t is piecewise smooth and, by Assumption 4.1, there exist a sequence $D_0, D_1, \ldots \in \mathbb{R}^{n_x \times n_u}$ and constants $C_H^0 \in \mathbb{R}$ and $C_H^1 \in \mathbb{R}_{++}$ such that

$$\log\left(\left\| H_t(\tau) - \sum_{i=0}^{M} D_i \Phi_i(\tau) \right\| \right) \le C_H^0 - C_H^1 M \tag{40}$$

for almost all $\tau \in [0,T]$ and all $M \in \mathbb{N}$. By combining (38) and (40), it follows that there exists a constant $C_\mu \in \mathbb{R}_{++}$ such that

$$\log\big(\mathrm{diam}\big(\mathbb{E}_M^{\mathrm{L}}(t,a)\big)\big) \le \log\left(2 \sup_c \frac{V(t,c)}{\|c\|_2} \right) \le 2C_\mu \big[C_H^0 - C_H^1 M \big] \tag{41}$$

for almost all $\tau \in [0,T]$ and all $M \in \mathbb{N}$. In the last step, we have used the Lebesgue dominated convergence theorem (or alternatively Fatou's lemma), which guarantees that the Lebesgue zero measure of points $\tau \in [0,T]$ at which inequality (40) may be violated does not contribute to the bound on the L_2-norm of the function $H_t - \sum_{i=0}^{M} D_i \Phi_i$. The statement of the theorem follows by taking $C_E^{L,0} := 2C_\mu C_H^0$ and $C_E^{L,1} := 2C_\mu C_H^1$. □

Finally, a proof of Theorem 4.1 is obtained by combining the results in Theorem A.1 and Lemma A.1.

Appendix B: Computation of Convergent Enclosures $\overline{\mathbb{E}}_M(t, \mathbb{A})$

Since the proof in Appendix A is essentially constructive, a line-by-line transcription of this proof into a numerical bounding procedure that constructs an enclosure $\overline{\mathbb{E}}_M(t, \mathbb{A})$ satisfying Assumption 5.2 is in principle possible, assuming that suitable interval tools are available. For the implementation in this paper, we have used the bounding and relaxation techniques available through the library MC++ [50, 58], and we have refined the procedure based on the following observations:

1. From inequality (39) we know that the set $\mathbb{E}_M^{\mathrm{L}}(t,a)$ is enclosed by an ellipsoid of the form $\mathcal{E}(Q(t,a))$ with

$$Q(t,a) := \int_0^T \left(H_t(\tau) - \sum_{i=0}^{M} \frac{\langle H_t, \Phi_i \rangle_\mu}{\sigma_i} \Phi_i(\tau) \right) \left(H_t(\tau) - \sum_{i=0}^{M} \frac{\langle H_t, \Phi_i \rangle_\mu}{\sigma_i} \Phi_i(\tau) \right)^{\mathsf{T}} \mathrm{d}\tau.$$

By using standard tools from interval analysis for differential equations, a convergent bounding matrix $\mathbb{Q}(t,\mathbb{A}) \in \mathbb{R}^{n_x \times n_x}$ can be constructed such that $Q(t,a) \preceq \mathbb{Q}(t,\mathbb{A})$ for all $a \in \mathbb{A}$ and all $t \in [0,T]$. In particular, if there exists a constant C_Q such that

$$\left\| \mathbb{Q}(t,\mathbb{A}) - \mathbb{Q}\big(t, \{\mathrm{mid}(\mathbb{A})\}\big) \right\| \le C_Q \,\mathrm{diam}(\mathbb{A}),$$

then the enclosure $\overline{\mathbb{E}}_M^{\mathrm{L}}(t,\mathbb{A}) := \mathcal{E}(\mathbb{Q}(t,\mathbb{A}))$ will satisfy the convergence conditions

$$\log\big(\mathrm{diam}\big(\overline{\mathbb{E}}_M^{\mathrm{L}}\big(t, \{\mathrm{mid}(\mathbb{A})\}\big)\big)\big) \le C_{\mathbb{E}}^{\mathrm{L},0} - C_{\mathbb{E}}^{\mathrm{L},1} M, \tag{42}$$

$$\mathrm{diam}\big(\overline{\mathbb{E}}_M^{\mathrm{L}}(t,\mathbb{A})\big) - \mathrm{diam}\big(\overline{\mathbb{E}}_M^{\mathrm{L}}\big(t, \{\mathrm{mid}(\mathbb{A})\}\big)\big) \le C_{\mathbb{E}}^{\mathrm{L},2}\, \mathrm{diam}(\mathbb{A}), \tag{43}$$

for all compact sets $\mathbb{A}$, for all $M \in \mathbb{N}$, and for some constants $C_{\mathbb{E}}^{\mathrm{L},0} \in \mathbb{R}$, $C_{\mathbb{E}}^{\mathrm{L},1} \in \mathbb{R}_{++}$, and $C_{\mathbb{E}}^{\mathrm{L},2} \in \mathbb{R}_{+}$.
2. The proof of Lemma A.1 is based on Gronwall's lemma, which is known to provide mathematically valid, yet typically conservative, bounds for practical purposes. Instead, our implementation considers a modified version of state-of-the-art reachable set enclosure algorithms for bounding the solution of the differential equation (33), which prove to be much less conservative than with Gronwall's lemma.

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