Reformulations and Algorithms for the Optimization of Switching Decisions in Nonlinear Optimal Control

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Abstract

In model-based nonlinear optimal control switching decisions that can be optimized often play an important role. Prominent examples of such hybrid systems are gear switches for transport vehicles or on/off valves in chemical engineering. Optimization algorithms need to take the discrete nature of the variables that model these switching decisions into account. Unnecessarily, for many applications still an equidistant time discretization and either rounding or standard mixed–integer solvers are used. In this article we survey recent progress in theoretical bounds, reformulations, and algorithms for this problem class and show how process control can benefit from them. We propose a comprehensive algorithm based on the solution of a sequence of purely continuous problems and simulations, and provide a new and more compact proof for its well-posedness. Instead of focusing on a particular application, we classify different solution behaviors in the applications section. We provide references to respective case studies with prototype character and cite newly emerging benchmark libraries. We conclude by pointing out future challenges for process control with switching decisions.

Key words: hybrid systems, optimal control, integer programming, MINLP

1. Introduction

We are interested in model-based nonlinear optimal control including switching decisions that are to be optimized together with continuous controls. For the sake of readability, we proceed as follows. We focus on a specific, simple case of such a mixed–integer optimal control problem (MIOCP) in ordinary differential equations (ODE) of the following form. Later on, in Section 7, we will discuss extensions to include different objective functionals, multi-point constraints, algebraic variables, more general hybrid systems, and the like. For now, we want to minimize a Mayer term

$$\min_{x,u,v} \Phi(x(t_{\mathrm{f}})) \tag{1a}$$

over the differential states $x(\cdot)$ and the control functions $(u, v)(\cdot)$ subject to the n_{x}-dimensional ODE system

$$\dot{x}(t) \quad = \quad f(x(t), u(t), v(t)), \qquad t \in [0, t_{\mathrm{f}}], \tag{1b}$$

fixed initial values

$$x(0) \quad = \quad x_0, \tag{1c}$$

a connected feasible domain for the continuous controls

$$u(t) \quad \in \quad \mathcal{U}, \qquad t \in [0, t_{\mathrm{f}}], \tag{1d}$$

and integrality of the control function $v(\cdot)$

$$v(t) \quad \in \quad \Omega := \{v^1, v^2, \ldots, v^{n_\omega}\}, \qquad t \in [0, t_{\mathrm{f}}]. \tag{1e}$$

The main focus of this paper lies on the control function $v(\cdot)$ that needs to take a value v^i from a finite set $\Omega \subset \mathbb{R}^{n_{\mathrm{v}}}$ at all times. In the following all functions are assumed to be sufficiently often continuously differentiable, and $\| \cdot \|$ will denote the maximum norm $\| \cdot \|_\infty$.

We will use the term *integer control* for (1e), while *binary control* refers to the special case $\omega(t) \in \{0, 1\}^{n_\omega}$. We use the expression *relaxed*, whenever a restriction $v(\cdot) \in \Omega$ is relaxed to a convex control set with a recently proposed outer convex relaxation [32] that we define as follows. For every element v^i of Ω a binary control function $\omega_i(\cdot)$ is introduced. The ODE (1b) can then be written as

$$\dot{x}(t) \quad = \quad \sum_{i=1}^{n_\omega} f(x(t), u(t), v^i)\, \omega_i(t), \qquad t \in [0, t_{\mathrm{f}}]. \tag{2}$$

If we impose the special ordered set type one condition

$$\sum_{i=1}^{n_\omega} \omega_i(t) \quad = \quad 1, \qquad t \in [0, t_{\mathrm{f}}], \tag{3}$$

there is obviously a bijection between every feasible integer function $v(\cdot) \in \Omega$ and an appropriately chosen binary function $\omega(\cdot) \in \{0,1\}^{n_\omega}$, compare Section 5.4. The relaxation of $\omega(t) \in \{0,1\}^{n_\omega}$ is given by $\omega(t) \in [0,1]^{n_\omega}$. The main focus of this paper lies on the control function $v(\cdot)$ that needs to take a value $v^i \in \Omega \subset \mathbb{R}^{n_\mathrm{v}}$. From another point of view, order and timing of switching between the v^i are to be determined.

Typical examples are the choice of gears in transport, [44], or processes with on/off valve positioning instead of pumps, [34, 18]. Note that an equivalent formulation that is sometimes used, especially in the hybrid systems community, is to write (1b, 1e) as

$$\dot{x}(t) \;=\; \tilde{f}_i(x(t), u(t)), \quad t \in [0, t_\mathrm{f}],\; 1 \le i \le n_\omega \tag{4}$$

as the choice of a model i to use.

There are three generic approaches to solve model-based optimal control problems, compare [5]. With its explicit approach, *Dynamic Programming* seems to be suited for a treatment of integer variables, but suffers in general from the so-called *curse of dimensionality* and is therefore not the method of choice for generic large–scale optimal control problems with underlying nonlinear differential (algebraic) equation systems. The same holds true for *indirect methods*, also known as the *first optimize, then discretize* approach, see Section 2. A main challenge stems from the complex intrinsic switching of the adjoint variables in the case of path constraints. However, to our knowledge the first MIOCPs ever were solved in the early eighties with this approach, [7]. Also, hybrid maximum principles have become an active field of research lately. Therefore we will present the basic ideas of Pontryagin's maximum principle and references in Section 2. The third generic approach, *direct methods* and in particular *all–at–once approaches*, have become the methods of choice for most practical problems, see [5]. We base most of the reformulations and algorithms on direct algorithms, hence we give an overview in Section 3.

Tackling generic problems of the form (1) is difficult because of the combined nonlinear and discrete nature. Several algorithms are capable of producing a sub-optimal solution with the strong property of integer feasibility. For these approaches a bound on the performance loss is of utmost importance. This will be addressed in Section 4. We first consider the case of linearly entering binary controls. In Sections 5.3 and 5.4 we will see how to obtain an equivalent formulation of this control-affine structure for (1).

Sections 5 and 6 list different approaches to overcome the intrinsic problem of direct approaches with integer variables, cumulating into a comprehensive algorithm in Section 6.4. As stated before, in Section 7 generalizations of the simple control problem (1) will be discussed. Instead of focusing on a particular application, we classify different solution behaviors in Section 8. We provide references to respective case studies with prototype character and cite newly emerging benchmark libraries. We conclude by pointing out future challenges for process control with switching decisions in Section 9.

2. Indirect approach to optimal control

The basic idea of indirect approaches is *optimize, then discretize.* In other words, first necessary conditions for optimality are applied to the optimization problem in function space, and in a second step the resulting boundary value problem is solved by an adequate discretization, such as multiple shooting. The necessary conditions for optimality are given by the famous Pontryagin's maximum principle. Assume we want to solve the following optimal control problem.

$$
\begin{array}{llll}
\min\limits_{x,w} & \Phi(x(t_\mathrm{f})) & & \\
\text{subject to} & & & \\
\quad \dot{x}(t) & = & f(x(t), w(t)), & t \in [0, t_\mathrm{f}], \\
\quad w(t) & \in & \mathcal{W}, & t \in [0, t_\mathrm{f}], \\
\quad x(0) & = & x_0, &
\end{array}
\tag{5}
$$

with an arbitrary, essentially bounded feasible set $\mathcal{W}$ for control $w(\cdot)$. To state the maximum principle we will need the concept of the Hamiltonian.

Definition 2.1. (Hamiltonian, adjoint states)
The Hamiltonian of optimal control problem (5) is given by

$$\mathcal{H}(x(t), w(t), \lambda(t)) \;:=\; \lambda(t)^T\, f(x(t), w(t))$$

with variables $\lambda : [t_0, t_f] \to \mathbb{R}^{n_x}$ called adjoint variables. The end–point Lagrangian function ψ is defined as $\psi(x(t_f)) := \Phi(x(t_f))$.

The *maximum principle* in its basic form, also sometimes referred to as *minimum principle*, goes back to the early fifties and the works of Hestenes, Boltyanskii, Gamkrelidze, and of course Pontryagin. Precursors of the maximum principle as well as of the Bellman equation can already be found in Carathéodory's book of 1935, compare [28] for details.

The maximum principle states the existence of adjoint variables $\lambda^*(\cdot)$ that satisfy adjoint differential equations and transversality conditions. The optimal control $w^*(\cdot)$ is characterized as an implicit function of the states and the adjoint variables — a minimizer $w^*(\cdot)$ of problem (5) also minimizes the Hamiltonian subject to additional constraints.

Theorem 2.2. (Maximum principle)
Let problem (5) have a feasible optimal solution $w^*(\cdot)$ with a system response $x^*(\cdot)$. Then there exist adjoint variables $\lambda^*(\cdot)$ such that for $t \in [0, t_f]$ it holds almost everywhere

$$\begin{aligned}
\dot{x}^*(t) &= \mathcal{H}_\lambda(x^*(t), w^*(t), \lambda^*(t)) = f(x^*(t), w^*(t)), && \text{(6a)}\\
\dot{\lambda}^{*T}(t) &= -\mathcal{H}_x(x^*(t), w^*(t), \lambda^*(t)), && \text{(6b)}\\
x^*(t_0) &= x_0, && \text{(6c)}\\
\lambda^{*T}(t_f) &= -\psi_x(x^*(t_f)), && \text{(6d)}\\
w^*(t) &= \arg\min_{w \in \mathcal{W}} \mathcal{H}(x^*(t), w(t), \lambda^*(t)). && \text{(6e)}
\end{aligned}$$

For a proof of the maximum principle and further references see, e.g., [9, 29]. The interesting part about the maximum principle is that the constraint $w(t) \in \mathcal{W}$ has been transferred towards the inner minimization problem (6e). This is done on purpose, so no assumptions need to be made on the feasible control domain $\mathcal{W}$. The maximum principle also applies to nonconvex and disjoint sets $\mathcal{W}$. Hence, if we write $w(\cdot) = (u, v)(\cdot)$ and $\mathcal{W} = \mathcal{U} \times \Omega$, the maximum principle also covers problem (1) and the inner minimization problem (6e) reads as

$$(u^*, v^*)(t) = \arg \min_{u \in \mathcal{U}, v \in \Omega} \mathcal{H}(x^*(t), u(t), v(t), \lambda^*(t)). \tag{7}$$

For a disjoint set Ω of moderate size the pointwise minimization of (7) can be performed by enumeration between the n_ω different choices, implemented as switching functions that determine changes in the minimum. This approach, the *Competing Hamiltonians* approach, has to our knowledge first been successfully applied to the optimization of operation of subway trains with discrete acceleration stages in New York by Bock and Longman [7].

Recently, additional work has been done on the formulation of more general results, in particular the *hybrid maximum principle*, [42], and a *hybrid necessary principle*, [15]. Furthermore, the proofs were simplified by making a direct connection to the classical maximum principle, [13]. Based on hybrid maximum principles or extensions of Bellman's equation approaches to treat switched systems have been proposed that extend indirect methods or dynamic programming, e.g., in [39, 1]. While the maximum principle and knowledge about solution behavior keeps being important for analytical reasons, see Section 8, direct methods have become the methods of choice for larger control problems of practical relevance in ordinary differential equations. It is interesting to observe, however, that this might be different in the case of partial differential equations (PDE). In the PDE constraint optimization community the two approaches *first optimize, then discretize* and *first discretize, then optimize* are still competing. One reasons for this is probably the fact that adjoints need to be determined for an efficient calculation of derivatives, which involves a second discretization grid for the backward solve. In higher dimensions the question which grid to choose becomes more important and favors an indirect approach. Also there is a tendency to treat spatial phenomena like shock waves rather in function space than by discretization, e.g., [12].

3. Direct approach to optimal control

The main idea of direct approaches is *first discretize, then optimize*. The control problem in a function space is discretized by means of parametric functions with local support, and then the resulting nonlinear program (NLP) in finitely many optimization variables is solved. There are basically three different approaches: *single shooting*, *Bock's direct multiple shooting*, and *collocation*. Details on these methods and how they relate to one another can be found, e.g., in [5, 2].

There are important differences between the approaches, mainly in the parameterization of the underlying differential equations and the respective connections to the optimization algorithm by means of derivative information. There are also good reasons why collocation and multiple shooting, both dating back to the early eighties, [6, 8, 3], are most often superior to the single shooting approach. However, all further algorithms and reformulations yet to be presented can be equally applied to any one of the three.

We restrict ourselves to a short presentation of the discretization of the respective functions in time, common to all three methods. Generally, any appropriate set of basis functions will do, e.g., splines or piecewise linear functions, if they can be described by means of finitely many values that will become the optimization variables. For the following it will be sufficient to assume a piecewise constant discretization of the form

$$\hat{u}(t, q_i^{\mathrm{u}}) \;:=\; q_i^{\mathrm{u}}, \quad \hat{v}(t, q_i^{\mathrm{v}}) := q_i^{\mathrm{v}}, \quad t \in [t_i, t_{i+1}] \tag{8}$$

on an appropriate time grid $0 = t_0 < t_1 < \ldots < t_m = t_{\mathrm{f}}$ and with control values $q_i^{\mathrm{u}} \in \mathbb{R}^{n_{\mathrm{u}}}$ and $q_i^{\mathrm{v}} \in \mathbb{R}^{n_{\mathrm{v}}}$. The control space is hence reduced to functions that can be written as in (8), depending on finitely many controls $(q^{\mathrm{u}}, q^{\mathrm{v}})$.

If present, also the path constraints $c(\cdot) \geq 0 \;\forall\; t \in [0, t_{\mathrm{f}}]$, compare Section 7, are discretized on an appropriately chosen grid. From this discretization and the (algorithm specific) parameterization of the differential states results a highly structured NLP that is usually solved by either an interior point or an active set based algorithm. For details on an efficient implementation and further references see, e.g., [24, 4].

If switching decisions or disjoint feasible sets are present as in (1e), the discretization (8) leads to control variables that inherit this integrality condition. For a piecewise constant discretization $q_i^{\mathrm{v}} \in \Omega$ needs to hold for all $0 \leq i < m$. Formally a mixed–integer nonlinear program is obtained.

4. Theory for control-affine systems

Most of the algorithms that have been applied to solve problem (1) cannot provide a rigorous lower bound on the optimal solution value. Even if global MINLP methods are applied, one does not know how good the solution really is, as the underlying control discretization grid might be too coarse in some regions or simply not hit the optimal switching points. Only recently the connection between rigorous bounds on the optimal integer solution value and results of relaxed, continuous control problems has been made, [32, 36].

Let us, for now, consider a *binary-control-affine problem* of the form

$$
\begin{array}{ll}
\min\limits_{x,u,\omega} & \Phi(x(t_\mathrm{f})) \\
\text{subject to} & \\
& \begin{array}{lcll}
\dot{x}(t) & = & \tilde{f}(x(t),u(t)) \cdot \omega(t), & t \in [0,t_\mathrm{f}], \\
u(t) & \in & \mathcal{U}, & t \in [0,t_\mathrm{f}], \\
\omega(t) & \in & \{0,1\}^{n_\omega}, & t \in [0,t_\mathrm{f}], \\
C(\omega(t)) & = & 0, & t \in [0,t_\mathrm{f}], \\
x(0) & = & x_0, &
\end{array}
\end{array}
\tag{9}
$$

with $\tilde{f} : \mathbb{R}^{n_\mathrm{x}} \times \mathbb{R}^{n_\mathrm{u}} \rightarrow \mathbb{R}^{n_\mathrm{x} \times n_\omega}$ and $C : \mathbb{R}^{n_\omega} \rightarrow \mathbb{R}^{n_C}$ an arbitrary constraint on the binary control. We will see later how the special case (9) relates to the more general problem (1) that we are really interested in. One of the observations in [32, 36] was that the optimal solution of the relaxation of control problem (9) yields the exact lower bound for (1), i.e., the value that can either be reached or be approximated arbitrarily close by an integer control. However, the proof used arguments from functional analysis and hence this result does not apply to a finite number of switches.

In [33] the statement was extended: for any $\delta > 0$ it holds that if the control discretization grid is chosen fine enough, then there exists a binary solution with a *finite number* of switches that yields an objective value closer than δ to the one of the relaxed problem. The basis for this is

Theorem 4.1. *Let $x(\cdot)$ and $y(\cdot)$ be solutions of the initial value problems*

$$\dot{y} = A(y) \cdot \alpha(t), \quad y(0) = y_0, \tag{10a}$$

$$\dot{x} = A(x) \cdot \omega(t), \quad x(0) = x_0 = y_0 \tag{10b}$$

with $t \in [0, t_f]$, for given functions $\alpha : [0, t_f] \rightarrow \mathbb{R}^{n_\omega}$ and $\omega : [0, t_f] \rightarrow \mathbb{R}^{n_\omega}$. If positive numbers $L, M, \epsilon \in \mathbb{R}^+$ exist such that for all $t \in [0, t_f]$ it holds that

$$\| \alpha(t) \| \leq 1, \quad \| \omega(t) \| \leq 1, \tag{10c}$$

$$\| A(x) \| \leq M \quad \forall\, x \in \mathbb{R}^{n_x}, \tag{10d}$$

$$\| A(y) - A(x) \| \leq L \| y - x \| \quad \forall\, x, y \in \mathbb{R}^{n_x}, \tag{10e}$$

$$\left\| \int_0^t \alpha(\tau) - \omega(\tau) \, \mathrm{d}\tau \right\| \leq \epsilon, \tag{10f}$$

then it also holds

$$\| y(t) - x(t) \| \leq \hat{M} \epsilon \tag{10g}$$

with constant $\hat{M} = 2Me^{Lt_f} - M$.

The relation between problem (9) and Theorem 4.1 is obvious. Let us assume we have found the feasible and optimal trajectory (x^*, u^*, α^*) of the relaxation of problem (9). We fix the continuous control functions $u^*(\cdot)$ and write the right hand side $f(x(\cdot), u(\cdot))\omega(\cdot)$ as a function $A(y(\cdot); u^*(\cdot))\omega(\cdot)$ of $y(\cdot)$ and $\omega(\cdot)$ only. The ODE in (9) is then in the form of (10b). We will see in Section 6.3 a constructive way to determine a binary control $\omega(\cdot)$ from $\alpha^*(\cdot)$ in a way that ϵ is a mere multiple of the control discretization grid size, and can hence be made arbitrarily small. This is done for two cases of interest: the one when there are no constraints, $C(\omega) = 0$, and when a special ordered set property $C(\omega) = \sum \omega_i - 1$ has to hold that stems from an equivalent reformulation of the general nonlinear case.

Theorem 4.1 now helps to estimate the performance loss between the optimal relaxed control $\alpha^*(\cdot)$ and the binary control $\omega(\cdot)$. As assumptions (10c) hold for both relaxed and binary controls, and assumptions (10d) and (10f) follow from a boundedness of the variable range for the differential states and from an assumed Lipschitz continuity, respectively, the difference between the differential states is determined from (10g), if (10f) holds. The Mayer function $\Phi(\cdot)$ is assumed to be differentiable, hence continuous. Therefore the difference between the objective function values of the original, binary control problem (9) and of its relaxation are bounded by a constant times ϵ.

The most interesting assumption of Theorem 4.1 is (10f). At first sight the condition is somewhat unusual, as one might expect an L^∞ norm,

$$\int_0^{t_\mathrm{f}} \| \, \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \, \| \quad \leq \quad \epsilon. \tag{11}$$

This condition is far too strong, however. While one direction is obvious,

$$\left\| \int_0^t \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \right\| \quad \leq \quad \int_0^t \| \, \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \, \| \leq \int_0^{t_\mathrm{f}} \| \, \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \, \|$$

one can construct an example for which the gap between the two expressions (10f) and (11) becomes as large as it can get. Assume an equidistant time grid $0 = t_0 < t_1 < \cdots < t_m = t_\mathrm{f}$, with $t_{i+1} - t_i = \frac{t_\mathrm{f}}{m}$. Define

$$\alpha(\tau) \quad := \quad \frac{1}{2}, \quad \omega(\tau) := \begin{cases} 1 & \tau \in [t_i, t_{i+1}], i \text{ even} \\ 0 & \tau \in [t_i, t_{i+1}], i \text{ odd} \end{cases}$$

We obtain

$$\int_0^{t_\mathrm{f}} \| \, \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \, \| \quad = \quad \frac{t_\mathrm{f}}{2} \quad \text{and} \quad \left\| \int_0^t \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \right\| \leq \frac{t_\mathrm{f}}{m},$$

where the second term vanishes for $m \to \infty$ for all $t \in [0, t_\mathrm{f}]$.

5. Reformulations

In the previous sections we developed both general methodology and theory that guarantees performance loss bounds for binary-control-affine systems. In this section we survey different reformulations. The first two, a switching time optimization approach in 5.1 and penalization strategies in 5.2, aim at producing sub-optimal integer feasible solutions. In subsections 5.3 and 5.4 the target is to reformulate the nonlinear problem equivalently to obtain a binary-control-affine system.

5.1. Switching Time Optimization

One possibility to solve problem (1) is motivated by the idea to optimize the switching times directly, and to take the values of the integer controls fixed on given intervals. This concept is old and well known from a) indirect approaches, where switching functions (derivatives of the Hamiltonian with respect to the controls) are used to determine switching times, from b) hybrid systems, where switching functions determine phase transitions, and from c) multi-stage processes, such as batch processes in chemical engineering, consisting of several phases with open duration, e.g., [23].

The main idea consists of a reformulation. The control $v(t)$ is fixed to a value $v^{i_j} \in \Omega$ on each interval $[t_j, t_j + 1]$, with an (a priori) fixed order of the v^{i_j}. The control problem to be solved reads as

$$\begin{array}{llll} \min\limits_{x,u,t_j} & \Phi(x(t_\mathrm{f})) & & \\ \text{subject to} & & & \\ \quad \dot{x}(t) & = & f(x(t), u(t), v^{i_j}), & t \in [t_j, t_{j+1}], \\ \quad u(t) & \in & \mathcal{U}, & t \in [0, t_\mathrm{f}], \\ \quad x(0) & = & x_0. & \end{array} \tag{12}$$

In practice one will not optimize the switching points t_j directly, but the scaled vector h of model stage lengths $h_j := t_{j+1} - t_j$, see [23, 17]. This approach is visualized in Figure 1 for a one-dimensional binary control. Although the algorithm looks very promising at first sight, it has some severe disadvantages. First, a nonregular situation that may occur when stage lengths are reduced to zero. Assume the length of an intermediate stage, say

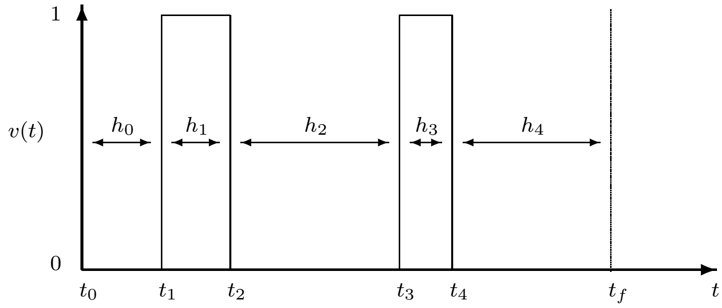

Figure 1: Switching time optimization, one–dimensional example.

h_2, has been reduced to zero by the optimizer. Then the sensitivity of the optimal control problem with respect to h_1 and h_3 is given by the value of their sum $h_1 + h_3$ only. Thus special care has to be taken to treat the case where stage lengths diminish during the optimization procedure. In [19], [20] and [25] an algorithm to eliminate such stages is proposed. This is possible, still the stage cannot be reinserted, as the time when to insert it is undetermined.

The second drawback is that the number of switches is typically not known, left alone the precise switching structure. Some authors propose to iterate on the maximum number of intervals until there is no further decrease in the objective function of the corresponding optimal solution, [19, 20, 25]. But it should be stressed that this can only be applied to more complex systems, if very good initial values for the location of all switching points are available. This is closely connected to the third and most important drawback of the switching time approach. The reformulation yields additional nonconvexities in the optimization space. Even if the optimization problem is convex in the optimization variables resulting from a constant discretization of the control function $v(\cdot)$, the reformulated problem may be nonconvex, compare[32].

The mentioned drawbacks of the switching time optimization approach can be overcome, though, if it is combined with a bunch of other concepts, compare [32, 17]. This includes good initial values, a strategy to deal with diminishing stage lengths and a direct all–at–once approach like direct multiple shooting that helps when dealing with nonconvexities as discussed in [32]. Also, making use of the theoretical results of Section 4, termination criteria for an iterative refinement of the switching structure need to be determined.

5.2. Reformulations to avoid integrality

The first idea to replace a binary variable $y \in \{0,1\}$ by a continuous variable $y \in [0,1]$ is to add the constraint $y\,(1-y) = 0$ to the problem formulation. Unfortunately this equality constraint is nonconvex with a disjoint feasible set and optimization solvers perform badly on such equations, as the necessary constraint qualification is violated.

Penalization strategies have the same aim as switching time optimization: working with continuous variables only, but obtaining an integer feasible solution. To do so for, say, the binary case $\omega(t) \in \{0,1\}^{n_\omega}$, we first relax towards $\omega(t) \in [0,1]^{n_\omega}$ for all $t \in [0, t_\mathrm{f}]$. To enforce a binary solution, we have two possibilities. One is to add a concave penalty function, e.g.,

$$\min_{x,u,\omega} \Phi(x(t_\mathrm{f})) + \sum_{i=1}^{n_\omega} \epsilon_i \int_{t_0}^{t_f} (1 - \omega_i(t))\, \omega_i(t)\, \mathrm{d}t$$

for $\epsilon_i \geq 0$. The other one would be to impose additional constraints,

$$(1 - \omega_i(t))\, \omega_i(t) \leq \epsilon_i \quad \forall\, t \in [0, t_\mathrm{f}].$$

An extension is to use a penalty term homotopy, by solving a series of continuous optimal control problems with relaxed $\omega(\cdot)$. One initializes problem P^{k+1} with the solution of P^k and raises ϵ_i^k until all $\omega_i(t)$ are 0 or 1.

Both approaches depend very much on the choice of ϵ and impose bad numerical behavior by either making the objective nonconvex, or splitting the feasible region into disjoint parts. Either approach may work well for special cases, but is generally not to be recommended. Details and a numerical case study can be found, e.g., in [32].

A clever problem-specific reformulation is proposed in [10, 11]. For the optimal operation of a water network the authors propose to *decompose the problem* in the sense that a pure NLP is solved for the overall network with a (continuous) aggregated output of the discrete-valued pumps in each waterworks. In a second step this optimal continuous output is approximated by solving a small-scale integer program for every waterworks in the system.

5.3. Reformulations to avoid nonlinearity

Another target for reformulations are the nonlinearities. We consider general linear approximations and products containing binary variables.

The basic idea to use underestimating and overestimating linear functions is best exemplified by replacing a bilinear term xy by a new variable z and additional constraints. This reformulation was proposed by [26]. For the new variable z we obtain the linear constraints

$$\begin{array}{rcccl} y^{\mathrm{lo}}x + x^{\mathrm{lo}}y - x^{\mathrm{lo}}y^{\mathrm{lo}} & \leq & z & \leq & y^{\mathrm{lo}}x + x^{\mathrm{up}}y - x^{\mathrm{up}}y^{\mathrm{lo}}, \\ y^{\mathrm{up}}x + x^{\mathrm{up}}y - x^{\mathrm{up}}y^{\mathrm{up}} & \leq & z & \leq & y^{\mathrm{up}}x + x^{\mathrm{lo}}y - x^{\mathrm{lo}}y^{\mathrm{up}}, \end{array} \tag{13}$$

for given bounds on x and y, i.e., $x \in [x^{\mathrm{lo}}, x^{\mathrm{up}}]$ and $y \in [y^{\mathrm{lo}}, y^{\mathrm{up}}]$. The inequalities follow from $(x - x^{\mathrm{lo}})(y - y^{\mathrm{lo}}) \geq 0$ and three similar equations. The snag is of course that very tight bounds are needed for a successful optimization, which is not the case in the presence of strong nonlinearities. See [43] or [14] for references on general under– and overestimation of functions. When binary variables enter in a nonlinear way into the right hand side function $f(\cdot)$, often simplifications are possible. All higher exponents can be skipped, as it holds $\omega_i(t) \cdot \omega_i(t) = \omega_i(t)$ for $\omega_i(t) \in \{0, 1\}$. Also for mixed products of binary variables a reduction of nonlinearity is possible. We introduce an additional variable, e.g., for $\omega_i(t) \cdot \omega_j(t)$:

$$\omega_{ij}(t) \quad := \quad \begin{cases} 1 & \text{if } \omega_i(t) = \omega_j(t) = 1 \\ 0 & \text{else} \end{cases}$$

The new binary variables can be incorporated into the optimization problem by adding the constraints

$$\omega_{ij}(t) \leq \omega_i(t), \quad \omega_{ij}(t) \leq \omega_j(t), \quad \omega_i(t) + \omega_j(t) \leq 1 + \omega_{ij}(t).$$

5.4. Outer convexification

We saw in Section 4 that for binary-control-affine models we get an estimate of the performance loss of any feasible binary solution by solving a relaxed problem. If nonlinearities with respect to the $v(\cdot)$ in (1) occur, they can sometimes be transformed as in Section 5.3. If this is not the case, a partial *outer convexification* with respect to the integer functions has been proposed in [32, 36]. Consider the following reformulation of problem (1),

$$\begin{array}{llll} \min\limits_{x,u,\omega} & \Phi(x(t_{\mathrm{f}})) & & \\ \text{subject to} & & & \\ \quad \dot{x}(t) & = & \sum_{i=1}^{n_\omega} f(x(t), u(t), v^i) \cdot \omega_i(t), & t \in [0, t_{\mathrm{f}}], \\ \quad u(t) & \in & \mathcal{U}, & t \in [0, t_{\mathrm{f}}], \\ \quad \omega(t) & \in & \{0, 1\}^{n_\omega}, & t \in [0, t_{\mathrm{f}}], \\ \quad \sum_{i=1}^{n_\omega} \omega_i(t) & = & 1, & t \in [0, t_{\mathrm{f}}], \\ \quad x(0) & = & x_0, & \end{array} \tag{14}$$

with fixed $v^i \in \Omega, 1 \leq i \leq n_\omega$. Problem (14) has two important properties: first, there is a bijection between solutions of (14) and of (1), hence any optimal solution is also optimal for the other problem. Second, it fits into the context of Section 4, as the binary controls enter linearly. In fact, as all v^i are fixed, problem (14) can be written in the form (9) with a matrix $\tilde{f}(\cdot)$ that contains $f(x(t), u(t), v^i)$ as its n_ω columns. There is one important modification: the additional linear constraint $0 = C(\omega) = \sum \omega_i - 1$ to ensure the controls form a special ordered set at each instant in time. This constraint needs to be taken into account whenever a binary solution is constructed from a relaxed one, compare Section 6.3.

Problem (14) yields a tight relaxation of the original problem (1). This reformulation comes at the price of additional control functions, as $v(\cdot)$ is replaced by n_ω controls $\omega_i(\cdot)$ (one less, if the linear equality constraint is used to eliminate one of them).

Note that depending on $f(\cdot)$, integer controls may decouple, leading to a reduced number n_ω. Assume we have

$$\begin{aligned} \dot{x}(t) &= g(\cdot, v_1(t)) + h(\cdot, v_2(t)), \\ v_1(t) &\in \Omega_1, \quad v_2(t) \in \Omega_2. \end{aligned}$$

Then an equivalent reformulation is given by

$$\begin{aligned} \dot{x}(t) &= \left(\sum_{i=1}^{n_{\omega_1}} g(\cdot, v_1^i)\, \omega_{1,i}(t) \right) + \left(\sum_{i=1}^{n_{\omega_2}} h(\cdot, v_2^i)\, \omega_{2,i}(t) \right), \\ \sum_{i=1}^{n_{\omega_1}} \omega_{1,i}(t) &= 1, \quad t \in [t_0, t_f], \\ \sum_{i=1}^{n_{\omega_2}} \omega_{2,i}(t) &= 1, \quad t \in [t_0, t_f], \\ \omega_1 &\in \{0,1\}^{n_{\omega_1}}, \quad \omega_2 \in \{0,1\}^{n_{\omega_2}}, \end{aligned}$$

leading to $n_\omega = n_{\omega_1} + n_{\omega_2}$ controls instead of $n_\omega = n_{\omega_1} n_{\omega_2}$. The proof is straightforward. As in most practical applications the binary control functions enter linearly (such as valves that indicate whether a certain term is present or not), or n_ω increases linearly with the number of choices (e.g., the gears), or integer controls decouple, the drawback of an increased number n_ω of control functions is clearly out-weighted by the advantages.

6. Algorithms

We present algorithms to solve problems of the form (1) and (14).

6.1. Rounding

One idea to solve problem (14) is to solve its relaxation (hence, $\omega(t) \in [0,1]^{n_\omega}$) and to round all $\omega_i(t)$ (alternatively their finite-dimensional parameterization q_i^ω) to the nearest binary value. In general mixed–integer programming this approach is not a good idea, rounded solutions are often very poor solutions or even infeasible. However, for control problems the optimal solution in function space is often of bang-bang type, i.e., the optimal control only takes values at its bounds. For these cases rounding performs well, if it is combined with an adaptive control discretization grid.

As follows from the results of Sections 4 and 5.4, we do have the exact lower bound from the solution of the relaxation of problem (14) and can hence estimate the performance loss associated with rounding. This is an important difference and advantage compared to general integer programming.

6.2. MI(N)LP algorithms

In the last 20 years important contributions in the field of algorithms for mixed–integer nonlinear programs (MINLPs) have been achieved. Of course both the classical algorithms Branch&Bound, Outer Approximation, and Bender's decomposition as newer developments including cutting planes and treatment of nonconvexities can be applied to the MINLP that stems from a discretization with a direct approach of problem (14).

If switching decisions or disjoint feasible sets are present as in (1e), discretization (8) leads to control variables that inherit this integrality condition. For a piecewise constant discretization $q_i^\omega \in \{0,1\}$ needs to hold for all i. The drawback of direct methods with integer control functions is obviously that they lead to high–dimensional vectors of binary/integer variables.

For many practical applications a fine control discretization is required. Therefore MINLP techniques will work only on limited and small time horizons because of the exponentially growing complexity of the problem, [45].

We recommend to use global MINLP algorithms only in two cases: first, when the control discretization grid is fixed and a global solution on this grid is of importance, and second, in an outer loop, when both integer control functions and non-time-dependent combinatorial decisions have to be made. In this case the problem can be decoupled, treating combinatorial decisions in an outer loop, and working with a relaxation of the integer control functions in the inner loop, compare Section 7.

6.3. Sum Up Rounding

A novel rounding strategy that is especially tailored to minimize expression (10f) on page 8 has first been proposed in the context of mixed-integer optimal control in [32]. We consider a piecewise constant control function

$$\alpha_j(t) = q^{\alpha}_{j,i} \in [0,1], \quad t \in [t_i, t_{i+1}] \tag{15}$$

with $j = 1 \dots n_\omega$ and $i = 0 \dots m-1$ on a fixed time grid $0 = t_0 < t_1 < \dots < t_m = t_f$, as introduced in Section 3. Such a function could be the result of an optimization with a direct approach that discretizes the control functions by piecewise constant functions. We write $\Delta t_i := t_{i+1} - t_i$ and Δt for the maximum distance between two time points,

$$\Delta t := \max_{i=0\dots m-1} \Delta t_i = \max_{i=0\dots m-1} \{t_{i+1} - t_i\}. \tag{16}$$

Let then a function $\omega(\cdot) : [0, t_f] \mapsto \{0,1\}^{n_\omega}$ be defined by

$$\omega_j(t) = p_{j,i}, \quad t \in [t_i, t_{i+1}] \tag{17}$$

where the $p_{j,i}$ are binary values given by

$$p_{j,i} \quad = \quad \begin{cases} 1 & \text{if } \sum_{k=0}^{i} q^{\alpha}_{j,k} \Delta t_k - \sum_{k=0}^{i-1} p_{j,k} \Delta t_k \geq 0.5 \Delta t_i \\ 0 & \text{else} \end{cases} . \tag{18}$$

See Figure 2 for an example. We have the following estimate on the integral over the difference between the control functions $\alpha(\cdot)$ and $\omega(\cdot)$.

Theorem 6.1. (Sum Up Rounding Integral Deviation)
Let the functions $\alpha : [0, t_f] \mapsto [0,1]^{n_\omega}$ and $\omega : [0, t_f] \mapsto \{0,1\}^{n_\omega}$ be given by (15) and (17, 18), respectively. Then it holds

$$\left\| \int_0^t \omega(\tau) - \alpha(\tau) \, \mathrm{d}\tau \right\| \leq 0.5 \; \Delta t.$$

For a proof see [33]. In combination with Theorem 4.1 this theorem allows us to relate the difference between differential states corresponding to any (relaxed) solution and a specific integer solution obtained by Sum Up Rounding to the size of the control discretization grid.

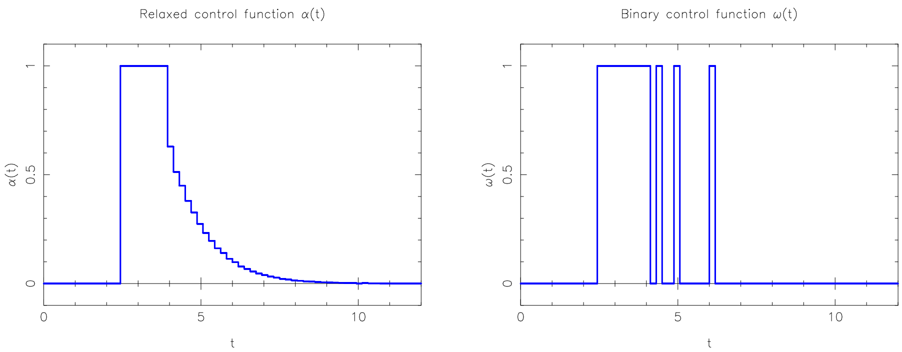

Figure 2: Relaxed and Sum Up Rounding binary controls for $m = 64$ time intervals.

Note that the Sum Up Rounding strategy (18) does not work for problems with the additional special ordered set property $\sum \omega_i = 1$ as in (14), as can be seen by the easy example of two functions that have the constant value $\alpha_1(t) = \alpha_2(t) = 0.5$. If we define $p_{j,i}$ to be

$$\hat{p}_{j,i} = \sum_{k=0}^{i} q^{\alpha}_{j,k} \Delta t_k - \sum_{k=0}^{i-1} p_{j,k} \Delta t_k \tag{19a}$$

$$p_{j,i} = \begin{cases} 1 & \text{if } \hat{p}_{j,i} \geq \hat{p}_{k,i} \; \forall \;\; k \neq j \text{ and } j < k \; \forall \;\; k : \hat{p}_{j,i} = \hat{p}_{k,i} \\ 0 & \text{else} \end{cases} \tag{19b}$$

a similar result to Theorem 6.1 holds, compare [33]. A related estimation of the discretization error can be found in the works of Veliov, e.g., [46].

6.4. MS MINTOC

We propose to use the following algorithm for the solution of (1). We denote the control discretization grid in iteration k with $\mathcal{G}^k$, and the optimal trajectory of (9) with $\mathcal{T}^k = (x^k(\cdot), u^k(\cdot), \alpha^k(\cdot))$. For the sake of notational simplicity we use $u^k(\cdot)$ and $\alpha^k(\cdot)$ and not the discretization variables $q^{\mathrm{u}}, q^{\alpha}$.

Algorithm 6.2. (MS MINTOC)

1. $k = 0$. *Input: initial control discretization grid* $\mathcal{G}^0$*, tolerance* $TOL \in \mathbb{R}^+$.
2. *If necessary, reformulate and convexify (Sections 5.3, 5.4) problem* (1). *Obtain problem of type* (9). *Relax this problem to* $\alpha(\cdot) \in [0, 1]^{n_\omega}$.
3. *REPEAT*
   (a) *Solve relaxed problem on* $\mathcal{G}^k$. *Obtain* $\mathcal{T}^k = (x^k(\cdot), u^k(\cdot), \alpha^k(\cdot))$ *and the grid–dependent optimal value* $\Phi^{REL}_{\mathcal{G}^k}$.

(b) *If* $\mathcal{T}^k$ *on* $\mathcal{G}^k$ *fulfills* $\omega^k(\cdot) := \alpha^k(\cdot) \in \{0,1\}^{n_\omega}$ *then STOP.*
(c) *Apply Sum Up Rounding (Section 6.3) to* $\alpha^k(\cdot)$*. Fix* $u^k(\cdot)$*.*
Obtain $y^k(\cdot)$ *and upper bound* $\Phi^{BIN}_{\mathcal{G}^k}$ *by simulation.*
(d) *If* $\Phi^{BIN}_{\mathcal{G}^k} < \Phi^{REL}_{\mathcal{G}^k} + TOL$ *then STOP.*
(e) *Refine the control grid* $\mathcal{G}^k$*.*
(f) $k = k + 1$*.*

4. *Bijection to obtain solution for problem* (1) *with objective* $\Phi^* = \Phi^{BIN}_{\mathcal{G}^k}$*.*

As for all algorithms we have to ask whether it is well-posed and will terminate in a finite number of steps. The answer is given by the following

Theorem 6.3. (Well-posedness of MS MINTOC)
If the assumptions

1. *On all grids* $\mathcal{G}^k$ *an optimal solution to the relaxed problem* (9) *is found in a finite number of operations.*
2. *Bisection is used for the refinement of* $\mathcal{G}^k$*.*
3. *After a finite number* k^{max} *of refinements we freeze the optimal relaxed solution,* $\mathcal{T}^k = \mathcal{T}^{k^{max}}$ *and* $\Phi^{REL}_{\mathcal{G}^k} = \Phi^{REL}_{\mathcal{G}^{k^{max}}}\ \forall\ k > k^{max}$*.*

hold, then Algorithm 6.2 will terminate in a finite number of steps with a feasible binary solution, for which $\Phi^* < \Phi^{REL}_{\mathcal{G}^k} + TOL$ *holds.*

Proof. By Assumption 1 all optimal control problems will be solved in finite time, and so will be the simulation in 3.(c). If the algorithm stops in 3.(b), a binary solution with $\Phi^* = \Phi^{\mathrm{REL}}_{\mathcal{G}^k}$ has been found. It is left to show that the algorithm will not loop infinitely often. Let $\omega^k(\cdot)$ be the control that we obtain from applying Sum Up Rounding on grid $\mathcal{G}^k$ to $\alpha^k(\cdot)$, and $y^k(\cdot)$ the vector of corresponding differential states. From Theorem 6.1 we have

$$\left\| \int_0^{t_\mathrm{f}} \omega^k(\tau) - \alpha^k(\tau)\ \mathrm{d}\tau \right\| \le 0.5\ \Delta t,$$

hence with Theorem 4.1 on page 8

$$\|\ y^k(t_\mathrm{f}) - x^k(t_\mathrm{f})\ \| \le M \Delta t e^{L t_\mathrm{f}}.$$

Due to Assumption 3, $x^k(\cdot)$ stays constant for $k \ge k^{\max}$. Reducing Δt by bisection will cause a strictly monotonic decrease of this expression, and this holds also for $\Phi(y^k(t_\mathrm{f})) - \Phi(x^k(t_\mathrm{f}))$, as $\Phi(\cdot)$ is a continuous function. □

Note that Algorithm 6.2 will be modified in practice for efficiency. Of particular interest are solutions with a small number of switches, but good performance. Therefore we recommend to include an intermediate switching time optimization (Section 5.1), initialized with the $\omega^k(\cdot)$ in 3.(c) to improve $\Phi^{\mathrm{BIN}}_{\mathcal{G}^k}$. It may also be advantageous to leave $u^k(\cdot)$ open for optimization, to compensate for the coarser grid. Also, adaptive refinements of the grid $\mathcal{G}^k$, based on control values $\alpha^k(\cdot)$ are preferable to bisection, see [32, 37].

7. More general problem classes

Problem (1) does not include all features that a mathematical model of a control process might show. In this section we discuss some straightforward extensions of the aforementioned approach, plus two features at the end, where special attention and further work is necessary.

Bolza type functionals. Every Lagrange term $\int L(x(t), u(t), v(t))\mathrm{d}t$ can be transformed equivalently into a Mayer term, hence the objective can also be of the more general Bolza type.
Multi-point constraints. Whenever multi-point constraints of the form

$$\begin{aligned} 0 &\leq r^{\mathrm{ieq}}(x(t_0), x(t_1), \ldots, x(t_{\mathrm{f}})), \\ 0 &= r^{\mathrm{eq}}(x(t_0), x(t_1), \ldots, x(t_{\mathrm{f}})) \end{aligned}$$

have to be fulfilled, the same argument as for the objective function can be used: All differential states corresponding to a relaxed solution can be approximated arbitrarily close by the ones corresponding to an integer solution, and $r^{\mathrm{ieq}}(\cdot), r^{\mathrm{eq}}(\cdot)$ are assumed to be at least continuous functions. Algorithm 6.2 needs to be extended in the sense that for all constraints an additional tolerance has to be checked in step 3.(d).
Path constraints. Path constraints $c(x(t), u(t)) \geq 0 \ \forall\ t \in [0, t_{\mathrm{f}}]$ are discretized in direct approaches, see Section 3, hence with a fixed $u^*(\cdot)$ the same argument as for multi-point constraints applies.
Time-independent continuous and combinatorial variables. For many processes also time-independent control values enter the problem formulation, say of continuous type, $p^{\min} \leq p \leq p^{\max}$, and of integer type, such as $\rho \in \{\rho^1, \rho^2, \ldots, \rho^{n_\rho}\}$. These control values are optimized together with the continuous controls $u^*(\cdot)$ and the relaxed binary controls $\alpha(\cdot)$. Once determined, $(u^*(\cdot), p^*, \rho^*)$ are fixed. In a second stage, the REPEAT loop of

Algorithm 6.2, feasible binary controls are determined. Especially integer control values ρ^* are typically hard to compute. Our procedure allows thus for a decoupling of the determination of optimal integer control values and optimal binary control functions, resulting in a huge reduction of complexity.

Multi-stage processes. Often complex practical processes, such as batch processes in chemical engineering or robot control, consist of several successive phases with different models and transition phases that may even change the number of differential states, see, e.g., [23]. The main additional effect of multiple stages that plays a role in Theorem 4.1 are the initial values of the differential states on each model stage determined by a continuous transition function. The expression $\| y_0^i - x_0^i \|$ for model stage i is nothing else than a function of the difference of the differential states on model stage $i-1$. Hence, also $\| y_0^i - x_0^i \|$ depends on the control discretization grid size Δt.

Global optimization. Algorithm 6.2 works for both global as local optimization. If a global method is applied in step 3.(a), the integer solution will approximate arbitrarily close the global optimum. If a local approach is chosen, the result is an approximation of this local optimum.

Multi-objective optimization. There is an important implication in the context of multi-objective optimization: whenever the Pareto front is to be calculated, it suffices to solve the relaxed convexified problem. The Pareto front of optimal control problems involving integer functions can hence be calculated without actually solving a single integer problem.

State-dependent switches. In hybrid systems a second type of discrete events may occur, namely state-dependent switches. Prominent examples are overflows in chemical engineering or ground contact in robotics, both dependent on a differential state (volume, vertical position) and triggering a model change. Mathematically these systems can be modeled by means of continuous switching functions. For all possible orderings of such events Theorems 4.1 and 6.1 can be adapted.

Algebraic variables and conditions. Theory and algorithms have to be extended for the case that algebraic equations involving the binary control functions are present, e.g., in an explicit system of index 1,

$$\begin{aligned} \dot{x}(t) &= f(x(t), z(t), u(t), \omega(t)), \quad t \in [0, t_\mathrm{f}], \\ 0 &= g(x(t), z(t), u(t), \omega(t)), \quad t \in [0, t_\mathrm{f}]. \end{aligned}$$

Formally, index 1 DAE systems can be transformed into an ODE, making it possible to treat them within the proposed methodology. However, for many systems special DAE solvers have been developed, as the additional derivation of the system is not beneficial from a numerical point of view. Further analysis is needed on how to exploit occurring structures.

(Mixed Path-) Control constraints. For generic constraints of the type

$$c(x(t), u(t), v(t)) \geq 0 \;\forall\, t \in [0, t_\mathrm{f}]$$

no termination criterium for Algorithm 6.2 can be guaranteed (think about a constraint that simply cuts off all binary solutions). Analysis must be problem or problem class specific and is a hot topic for future research. One general idea is to reformulate the constraints for $t \in [0, t_f], j = 1, \ldots, n_\omega$ to

$$0 \;\; \leq \;\; c(x(t), u(t), v^j) \;\; \omega_j(t). \tag{20}$$

Note that by constraint (20) only positive relaxed solutions are feasible, for which also the corresponding binary vector is feasible. This makes it more unlikely (although not impossible) that the index j corresponding to a value $q^\alpha_{j,i} = 0$ is chosen as the maximum in (19), whenever $c(x(t), u(t), v^j) < 0$ on $[t_i, t_{i+1}]$. Furthermore this constraint should be included in the rounding decision to avoid infeasibilities. Investigating this approach more rigorously is beyond the scope of this paper, however.

8. Applications

Instead of going into the details of a particular application involving switching decisions to be optimized, we survey and classify already published control problems. The intention is to provide modelers with an overview of existing hybrid system models with switching decisions to ease the modeling process, and to make a first step towards a benchmark library in the sense of netlib, miplib, minlplib, and the like for MIOCPs. Several examples can be found on the [27] website, although, unfortunately, most problems lack a precisely defined scenario including initial values, exact objective function, and all model parameters. A new effort in this direction is the MINTOC webpage, [31], a benchmark library in Wiki form.

The classification we propose for switching decisions is based on insight from Pontryagin's maximum principle, see Section 2, applied here only to the relaxed binary control functions $\alpha(\cdot)$. In the analysis of linear control problems one distinguishes three cases: bang-bang arcs, sensitivity-seeking arcs, and path-constrained arcs, [41], where an arc is defined to be a nonzero time-interval. Of course a problem's solution can show two or even all three behaviors at the same time on different arcs.

Bang-bang arcs. The case where the optimal solution contains only bang-bang arcs (time intervals on which $\alpha_i(t) \in \{0, 1\}\ \forall\, i$) is in a sense the easiest. The main goal will be to adapt the control discretization grid such that Algorithm 6.2 finally terminates in step 3.(b). A prominent example of this class is time-optimal car driving. In [16, 17, 21, 35] numerical results for extended benchmark problems have been deduced. The outer convexification approach (Section 5.4) led to a tremendous speed-up compared to the published reference benchmark solution for a fixed control discretization grid by several orders of magnitude as shown in Table 1. In [21] one can also find an explanation why a bang-bang solution for the relaxed and convexified gear choices has to be optimal. Further examples of "bang-bang solutions" include

	Inner convexification and Branch&Bound		**Outer convexification and MS MINTOC**	
m	t_f	CPU Time	t_f	CPU Time
20	6.779751	00:23:52	6.779035	00:00:24
40	6.786781	232:25:31	6.786730	00:00:46
80	–	–	6.789513	00:04:19

Table 1: Comparison of computational times for a Branch&Bound approach on a Pentium III machine with 750 MHz, [16] (left), and for MS MINTOC on an AMD Athlon XP 3000+ with 2.166 GHz, [21] (right). m denotes the number of control discretization intervals, t_f is the optimal objective function value. The path constraints are discretized on the same grid, hence the non-monotonicity of t_f in m. CPU times are given in hh:min:sec. Note that the results based on MS MINTOC were obtained on a computer that is approximately 4 times faster than the Pentium III machine, which would normally make a comparison of computation times highly suspect. However, here the computation times vary by at least 2 orders of magnitude with a difference growing in m, which is clearly a significant improvement even with the difference in machines.

free switching of ports in Simulated Moving Bed processes, [18, 34], time-dependent tray selection in batch distillation processes [32], unconstrained energy-optimal operation of subway trains [36], a simple F-8 flight control problem [20, 32], optimal transit path determination for a submarine vessel [30], and phase resetting in biological systems [22, 40, 38].

Path–constrained arcs. Whenever a path constraint is active, i.e., it holds $c_i(x(t)) = 0\ \forall\, t \in [t^{\mathrm{start}}, t^{\mathrm{end}}] \subseteq [0, t_\mathrm{f}]$, and no continuous control $u(\cdot)$ can be

Optimal solution with 1 touch point   Optimal solution with 3 touch points

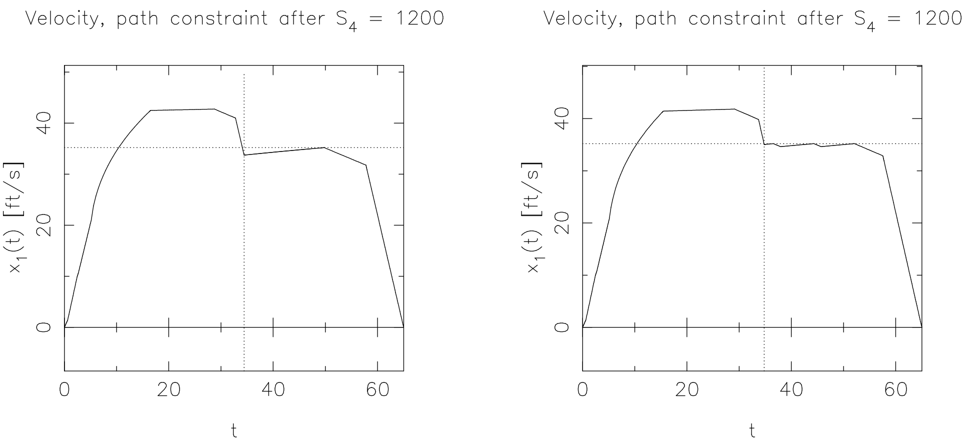

Figure 3: The differential state *velocity* of a subway train over time. The dotted vertical line indicates the beginning of the path constraint, the horizontal line the maximum velocity. Left: one switch leading to one touch point. Right: optimal solution for three switches. The energy-optimal solution needs to stay as close as possible to the maximum velocity on this time interval to avoid even higher energy-intensive accelerations in the start-up phase to match the terminal time constraint $t_{\mathrm{f}} \leq 65$ to reach the next station.

determined to compensate for the changes in $x(\cdot)$, naturally $\alpha(\cdot)$ needs to do so by taking values in the interior of its feasible domain. An illustrating example has been given in [36], where velocity limitations for the energy-optimal operation of New York subway trains are taken into account. The optimal integer solution does only exist in the limit case of infinite switching (Zeno behavior), or when a tolerance is given. Algorithm 6.2 will then terminate in step 3.(d) with a solution that approximates the optimal driving behavior (a convex combination of two operation modes) by switching between the two and causing a touching of the velocity constraint from below as many times as we switch, see Figure 3. Another example is compressor control in supermarket refrigeration systems, [27]. Note that all applications may comprise path-constrained arcs, once path constraints need to be added.

Sensitivity–seeking arcs. A classical small-sized benchmark problem for a sensitivity-seeking arc is the Lotka-Volterra Fishing problem, [32]. The optimal relaxed control calculated with a direct approach and approximating the solution on this arc is shown in Figure 2. As above, Algorithm 6.2 will terminate in step 3.(d) once the a priori specified tolerance has been reached, probably at the price of frequent switching. Further examples for sensitivity–seeking arcs are sliding mode control and the famous example of Fuller, [32].

9. Summary and Outlook

We presented a broad overview on recent mathematical developments in the efficient algorithmic treatment of switching decisions in nonlinear optimal control, meant to redefine the state of the art in this active field of research in process control. Theoretical foundations for error estimates are given alongside a discussion of possible solution approaches. A comprehensive algorithm is presented. Well-posedness of the algorithm is discussed, as well as extensions to treat more general optimal control problems. For the first time a classification of MIOCPs is presented based on analytical insight.

Future work in this field will focus on the efficient inclusion of algebraic variables, on problem specific analysis of control constraints, and on extensions in the context of robust and online optimization. The benchmark library [31] intends to deliver an open platform for algorithm developers, participation and contributions are very welcome.

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