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Switching Time Optimization for Bang-Bang and Singular Controls

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Abstract Optimal control problems with the control variable appearing linearly are studied. A method for optimization with respect to the switching times of controls containing both bang-bang and singular arcs is presented. This method is based on the transformation of the control problem into a finite-dimensional optimization problem. Therein, first and second-order optimality conditions are thoroughly discussed. Explicit representations of first and second-order variational derivatives of the state trajectory with respect to the switching times are given. These formulas are used to prove that the second-order sufficient conditions can be verified on the basis of only first-order variational derivatives of the state trajectory. The effectiveness of the proposed method is tested with two numerical examples.

Keywords Bang-bang control · Singular control · Second-order sufficient conditions · Variational derivatives

1 Introduction

Second-order sufficient conditions (SSC) have extensively been studied for problems where the control variable enters the system nonlinearly, cf., e.g., Maurer [1], Pickenhain [2], Zeidan [3] and many more. In these papers, one basic assumption is that the strict Legendre-Clebsch condition is satisfied which precludes the direct application of these methods to bang-bang and singular controls. Other approaches involve the technique of regular synthesis (cf., Boltyanskii [4] and Piccoli/Sussmann [5]) and the method of characteristics (cf., Noble/Schättler [6]). Agrachev et al. [7]

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and Osmolovskii/Maurer [8, 9] have developed SSC for bang-bang controls which involve the so–called induced optimization problem. This approach is based on optimization with respect to the switching times of the control, the free initial values of the states and the free final time. SSC for purely (often called totally) singular controls have been developed by Dmitruk [10]. Until now, only a few work on SSC for controls which are a concatenation of bang-bang and singular arcs has been published, cf., Piccoli/Sussmann [5], Poggiolini/Stefani [11] and Vossen [12]. Such controls shall be called bang-singular controls. We point out one crucial difference between bang-bang and bang-singular scalar controls. The sufficient conditions by Agrachev et al. [7], Osmolovskii/Maurer [8, 9] and Noble/Schättler [6] for bang-bang controls are restricted to controls where the total time derivative of the corresponding switching function is nonzero at the switching times. Contrary to that situation, we will investigate bang-singular controls. Here, the total time derivative of the switching function vanishes at the transition points between bang-bang and singular arc.

The organization of this paper is as follows: In Sect. 2, the statement of the problem and the known necessary optimality conditions from the Pontryagin minimum principle [13] are given. Section 3 introduces the induced optimization problem for bang-singular controls to optimize the (finitely many) control discontinuity points, the free initial state values and the free final time for a fixed control structure, i.e., a fixed sequence of bang-bang and singular arcs in feedback form. This method is an improvement of the known induced optimization problem for bang-bang controls.

First and second-order optimality conditions for the induced optimization problem are investigated in Sect. 4. Variational derivatives of the state trajectory and the Lagrangian function are given explicitly. The main result of this section is that the verification of second-order sufficient conditions requires the computation of only first-order variational derivatives of the states, cf., the ideas in Osmolovskii/Maurer [8, 9] for bang-bang controls. Due to limited space in this article, we refer to Vossen [14] for detailed proofs of all results in this section.

In Sect. 5, our method will be applied to two numerical examples, the optimal control of a van der Pol oscillator and the famous Goddard problem, see Bryson/Ho [15] and Maurer [16]. In both examples, the control structure is obtained via the software package IPOPT by Wächter/Biegler [17] whereas the induced problem is implemented using the code NUDOCCCS by Büskens [18]. A comparison with other methods will also be presented.

Second-order sufficient conditions in the induced problem for bang-bang controls together with certain regularity conditions imply optimality of the trajectory in the class of all admissable controls, cf., Agrachev et al. [7] and Osmolovskii/Maurer [8, 9]. Since no such result is known for controls with singular arcs we can show sufficient conditions in the class of controls with the same switching structure.

2 Statement of the Problem and Necessary Optimality Conditions

We consider the following class of optimal control problems in Mayer form, where $x(t) \in \mathbb{R}^n$ denotes the state variable and $u(t) \in \mathbb{R}^m$ the control variable in the time interval $[0, t_f]$ with the final time $t_f > 0$ being fixed or free:

$$\min \quad g(x(0), x(t_f), t_f), \tag{1}$$

$$\text{s.t.} \quad \dot{x}(t) = f(t, x(t), u(t)) = f_1(t, x(t)) + f_2(t, x(t))u(t) \quad \forall t \in [0, t_f], \tag{2}$$

$$\phi(x(0), x(t_f), t_f) = 0, \tag{3}$$

$$u(t) \in U \quad \forall t \in [0, t_f]. \tag{4}$$

Here, $g : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is a scalar function, $\phi : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^r$, $0 \le r \le 2n + 1$, and $f_1 : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ are column-vector functions, whereas $f_2 : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^{n,m}$ is a matrix function. The functions f_1, f_2, g and ϕ are assumed to be twice continuously differentiable. For simplicity, we suppose that the control set is the cube

$$U := [u_1^{\min}, u_1^{\max}] \times \cdots \times [u_m^{\min}, u_m^{\max}], \qquad u_k^{\min} < u_k^{\max}, \quad k = 1, \ldots, m. \tag{5}$$

We use the abbreviations

$$x_0 := x(0), \qquad x_f := x(t_f), \qquad x_b := (x_0, x_f).$$

A pair of functions $\mathcal{T} := (x(\cdot), u(\cdot))$ is said to be *admissible*, if $x(\cdot)$ is absolutely continuous, $u(\cdot)$ is measurable and essentially bounded and the pair of functions $\mathcal{T}$ satisfies the constraints (2)–(4). The component $x(\cdot)$ is called *state trajectory*.

First-order necessary optimality conditions for problem (1)–(4) are given by the Pontryagin minimum principle. The Pontryagin or Hamiltonian function is defined by

$$H(t, x, u, \lambda) := \lambda f(t, x, u) = \lambda f_1(t, x) + \lambda f_2(t, x)u,$$

where $\lambda \in \mathbb{R}^n$ is a row vector and is referred to as the *adjoint variable*. The factor of u in the Hamiltonian is called the *switching vector*

$$\sigma(t, x, \lambda) := (\sigma_1(t, x, \lambda), \ldots, \sigma_m(t, x, \lambda)) := \lambda f_2(t, x) \in \mathbb{R}^m. \tag{6}$$

We introduce the Lagrangian function for the initial and terminal point, the

$$l(x_b, t_f, \rho_0, \rho) := \rho_0 g(x_b, t_f) + \rho\phi(x_b, t_f),$$

with multipliers $\rho_0 \in \mathbb{R}$ and a row vector $\rho \in \mathbb{R}^r$. In the sequel, the partial derivatives of functions will be denoted by subscripts referring to the respective variables. The following necessary optimality conditions by Pontryagin et al. [13] are well-known.

If $\hat{\mathcal{T}} := (\hat{x}(\cdot), \hat{u}(\cdot))$ provides a minimum for the problem (1)–(4), then there exist an absolutely continuous function $\lambda : [0, t_f] \to \mathbb{R}^n$ and multipliers $\rho_0 \ge 0$ and $\rho \in \mathbb{R}^r$ that satisfy the following conditions:

$$\dot{\lambda}(t) = -H_x(t, \hat{x}(t), \hat{u}(t), \lambda(t)), \tag{7}$$

$$\lambda(0) = -l_{x_0}(\hat{x}(0), \hat{x}(\hat{t}_f), \hat{t}_f, \rho_0, \rho), \tag{8}$$

$$\lambda(\hat{t}_f) = l_{x_f}(\hat{x}(0), \hat{x}(\hat{t}_f), \hat{t}_f, \rho_0, \rho), \tag{9}$$

$$\frac{d}{dt}H(t,\hat{x}(t),\hat{u}(t),\lambda(t)) = H_t(t,\hat{x}(t),\hat{u}(t),\lambda(t)), \tag{10}$$

$$H(\hat{t}_f,\hat{x}(\hat{t}_f),\hat{u}(\hat{t}_f),\lambda(\hat{t}_f)) = -l_{t_f}(\hat{x}(0),\hat{x}(\hat{t}_f),\hat{t}_f,\rho_0,\rho), \quad \text{if } t_f \text{ is free}, \tag{11}$$

$$H(t,\hat{x}(t),\hat{u}(t),\lambda(t)) = \min_{u\in U} H(t,\hat{x}(t),u,\lambda(t)). \tag{12}$$

Equation (7) is called *adjoint differential equation*, conditions (8) and (9) are called *transversality conditions*, whereas (12) is called *minimum condition*. Henceforth, we use the notations

$$f(t) = f(t,x(t),u(t)), \qquad \sigma(t) = \sigma(t,x(t),\lambda(t)) = (\sigma_1(t),\dots,\sigma_m(t)), \quad \text{etc.},$$

along an admissible trajectory that satisfies the conditions (7)–(12). Evaluating the minimum condition (12) for the admissible control set U in (5), we get the following control law for the kth control component:

$$\hat{u}_k(t) = \begin{cases} u_k^{\min}, & \text{if } \sigma_k(t) > 0, \\ u_k^{\max}, & \text{if } \sigma_k(t) < 0, \\ \text{undetermined}, & \text{if } \sigma_k(t) = 0. \end{cases} \tag{13}$$

Definition 2.1 (Bang-Bang and Singular Controls, Switching Times) Consider an optimal trajectory $\hat{\mathcal{T}} = (\hat{x}(\cdot),\hat{u}(\cdot))$ and $0 \le t_1 < t_2 \le \hat{t}_f$. The control component $\hat{u}_k(t)$, $1 \le k \le m$, is called *bang-bang* on $[t_1,t_2]$ if $\sigma_k(t)$ has only isolated zeros on $[t_1,t_2]$. In this case, the optimal control component $\hat{u}_k(t)$ fulfills

$$\hat{u}_k(t) \in \{u_k^{\min}, u_k^{\max}\}, \quad \forall t \in [t_1,t_2].$$

We denote the control component $\hat{u}_k(t)$ as *singular* on $[t_1,t_2]$ if

$$\sigma_k(t) \equiv 0, \quad \forall t \in [t_1,t_2]$$

holds. A point $t_1 \in (0,\hat{t}_f)$ is called *switching time* if, for some $k \in \{1,\dots,m\}$,

(i) $\sigma_k(t)\sigma_k(t') < 0$ for all $t \in I_\epsilon^-$, $t' \in I_\epsilon^+$, or
(ii) $\sigma_k(t) \equiv 0$ on either I_ϵ^- or I_ϵ^+,

where $I_\epsilon^- = (t_1-\epsilon,t_1)$ and $I_\epsilon^+ = (t_1,t_1+\epsilon)$, with $\epsilon > 0$ sufficiently small.

Remark 2.1 In other words, a switching time t_1 is a transition point between one bang-bang arc and another bang-bang (case (i)) or a singular (case (ii)) arc. Clearly, this definition implies $\sigma_k(t_1) = 0$ as $\sigma_k(t)$ is continuous.

Switching law (13) implies that the optimal control $\hat{u}$ may be discontinuous at a switching time. Note that the set of all discontinuity points of $\hat{u}$ often exactly coincides with the set of all switching times, cf., Remark 3.1 in Sect. 3.

In this paper, we consider only controls with finitely many discontinuity points, cf., Assumption 3.1 in Sect. 3 and the discussions afterwards. We use the following notations for functions with discontinuity points.

Definition 2.2 Let $\mathcal{F} : [0, t_f] \to \mathbb{R}^{\dim \mathcal{F}}$ be continuous on $[0, t_f] \setminus \theta$ where $\theta := \{t_1, \ldots, t_d\}$ is the set of discontinuities of $\mathcal{F}$. We denote the left-hand respectively right-hand limit of $\mathcal{F}$ on $[0, t_f]$ as

$$\mathcal{F}(t^-) := \lim_{s\uparrow t} \mathcal{F}(s), \qquad \mathcal{F}(t^+) := \lim_{s\downarrow t} \mathcal{F}(s).$$

On θ, we shall use the notations

$$\mathcal{F}^{i-} := \mathcal{F}(t_i^-), \qquad \mathcal{F}^{i+} := \mathcal{F}(t_i^+), \qquad [\mathcal{F}]^i := [\mathcal{F}(t_i)] := \mathcal{F}^{i+} - \mathcal{F}^{i-}$$

for the left-hand and right-hand limit of $\mathcal{F}$ in t_i and for the jump of $\mathcal{F}$ in t_i, $i \in \{1, \ldots, d\}$, respectively.

The following quantities were introduced by Milyutin/Osmolovskii [19].

Definition 2.3 On the set $\theta = \{\hat{t}_1, \ldots, \hat{t}_d\}$ of discontinuity points of the optimal control $\hat{u}$, we define for $i = 1, \ldots, d$

$$(\Delta_i H)(t) := H(t, \hat{x}(t), \hat{u}^{i+}, \lambda(t)) - H(t, \hat{x}(t), \hat{u}^{i-}, \lambda(t)) = \sigma(t)[\hat{u}]^i,$$
$$D^i(H) := -\frac{d}{dt}(\Delta_i H)(\hat{t}_i).$$

Corollary 2.1 *The quantity $D^i(H)$ satisfies*

$$\begin{aligned} D^i(H) &= -[H_t]^i - [H_x]^i f^{i+} + H_x^{i+}[f]^i = -\dot{\sigma}^{i+}[\hat{u}]^i \\ &= -[H_t]^i - [H_x]^i f^{i-} + H_x^{i-}[f]^i = -\dot{\sigma}^{i-}[\hat{u}]^i \geq 0. \end{aligned} \tag{14}$$

A proof is given in [19]. Bang-bang controls, where the inequality holds strictly, are called regular bang-bang controls [8, 9] and arise in many applications. On the other hand, we now present a condition for bang-singular controls.

Corollary 2.2 *Let $\hat{u}$ be discontinuous at $\hat{t}_i$ for exactly one component $\bar{k} \in \{1, \ldots, m\}$ and let $\hat{u}_{\bar{k}}$ be singular on $[\hat{t}_i - \epsilon, \hat{t}_i]$ or $[\hat{t}_i, \hat{t}_i + \epsilon]$ for some sufficiently small $\epsilon > 0$. Then, $D^i(H) = 0$ holds.*

Proof We consider $\bar{k} = 1$. As $u_2, \ldots, u_m$ are continuous at $\hat{t}_i$, (14) yields

$$D^i(H) = -\dot{\sigma}_1^{i+}[\hat{u}_1]^i = -\dot{\sigma}_1^{i-}[\hat{u}_1]^i.$$

The last equality implies $\dot{\sigma}_1^{i+} = \dot{\sigma}_1^{i-}$ since $\hat{u}_1$ is discontinuous at $\hat{t}_i$. Since furthermore $\hat{u}_1$ is singular on $[\hat{t}_i - \epsilon, \hat{t}_i]$ or $[\hat{t}_i, \hat{t}_i + \epsilon]$, we have $\dot{\sigma}_1^{i-} = 0$ or $\dot{\sigma}_1^{i+} = 0$, which means $\dot{\sigma}_1^{i-} = \dot{\sigma}_1^{i+} = 0$ and $D^i(H) = 0$. □

3 Induced Optimization Problem

Assuming that the optimal control structure is known, we are going to formulate a new finite-dimensional optimization problem involving the initial states, the switching times and the final time t_f as optimization variables. In applications one can often obtain the control structure by using a direct method, i.e., discretizing the problem and solving the high-dimensional nonlinear optimization problem. Another idea is to guess a possible control structure and start with some additional bang-bang and singular arcs. The optimization approach will then lead to a solution where the lengths of all redundant arcs will be optimized to zero. Alternatively, the direct monotone structural evolution method by Szymkat/Korytowski [20] additionally takes advantage of the minimum principle optimality conditions to obtain the correct control structure. While this paper was under review, Szymkat and Korytowski were working on further improvements of their method using first- and second-order variational derivatives with respect to the switching times.

3.1 Basic Assumptions

The induced optimization problem is formulated under the following three assumptions for the optimal trajectory $\hat{\mathcal{T}} = (\hat{x}(\cdot), \hat{u}(\cdot))$, which hold in many applications.

Assumption 3.1 The optimal control $\hat{u}$ has finitely many switching times

$$0 =: t_0 < \hat{t}_1 < \cdots < \hat{t}_d < \hat{t}_{d+1} := \hat{t}_f.$$

Here and in the following, $d < \infty$ denotes the number of switching times.

Assumption 3.2 If $\hat{u}_k$ is singular on $[\hat{t}_{i-1}, \hat{t}_i]$, then $u_k^{\min} < \hat{u}_k(t) < u_k^{\max}$ holds for all $t \in [\hat{t}_{i-1}, \hat{t}_i]$. In other words, the control takes boundary values of the control set only on the bang-bang arcs and is in particular discontinuous at all switching times.

Assumption 3.3 In each interval $(\hat{t}_{i-1}, \hat{t}_i),\ i = 1, \ldots, d+1$, the control u can be obtained in *feedback form*, i.e., there exists a twice continuously differentiable function $u^i(t, x)$, such that the control is given by

$$\hat{u}(t) = u^i(t, \hat{x}(t)), \quad \forall t \in (\hat{t}_{i-1}, \hat{t}_i). \tag{15}$$

Remark 3.1 Assumption 3.3 in particular implies that $\hat{u}(t)$ is continuous on each interval $(\hat{t}_{i-1}, \hat{t}_i)$. Hence, Assumption 3.2 ensures that the discontinuity points of $\hat{u}$ coincide exactly with the switching times.

It is easy to verify Assumptions 3.1 and 3.2 for a given control $u(t)$. However, for Assumption 3.3 we will now present a method which, in many cases, provides the feedback form (15). At the end of this section, we furthermore present some ideas on how to deal with problems where Assumption 3.3 does not hold.

If the component $\hat{u}_k$, $1 \le k \le m$, is bang-bang along $[\hat{t}_{i-1}, \hat{t}_i]$, then either $u_k^i(t, x) \equiv u_k^{\min}$ or $u_k^i(t, x) \equiv u_k^{\max}$ yields the feedback expression (15). For a singular control component, the following method can be used. If the control is scalar, i.e. $m=1$, the control variable often appears in a certain, say pth, time derivative of the switching function in the following form:

$$\frac{d^p}{dt^p}\sigma(t,\hat{x}(t),\lambda(t)) = A(t,\hat{x}(t),\lambda(t)) + B(t,\hat{x}(t),\lambda(t))\hat{u}(t) \equiv 0, \tag{16}$$

with a coefficient $B(t,\hat{x}(t),\lambda(t)) \neq 0$ for all $t \in [\hat{t}_{i-1},\hat{t}_i]$, where p is an even number with $p=2q$ and q is called the order of the singular control, see Kelley/Kopp/Moyer [21], Bell/Jacobson [22] or Fraser-Andrews [23]. Solving (16) for u leads to a function $u(t,x,\lambda)$ where the component λ can often be eliminated due to

$$\frac{d^j}{dt^j}\sigma(t,\hat{x}(t),\lambda(t)) \equiv 0, \quad j=0,\dots,p-1.$$

Note that the classical junction theorem by McDanell/Powers [24] excludes the case that q is even, since Assumptions 3.1 and 3.2 cannot be fulfilled simultaneously. For vector-valued controls, the order of the singular control can be defined in the same way. The order q_k of a singular control component $\hat{u}_k$ is given by $2q_k = p_k$. Here, p_k is the lowest order time derivative of σ_k where u_k occurs with a coefficient not identically zero. Krener [25] has shown that p_k is even and hence $q_k \in \mathbb{N}$. Note that other control components u_l, $l \neq k$, can occur in the time derivatives of the switching function σ_k. However, the coefficients of certain singular components u_l vanish along an optimal trajectory due to the first generalized Legendre-Clebsch condition [25],

$$\frac{\partial}{\partial u_l}\left(\frac{d^j}{dt^j}\sigma_k(t,\hat{x}(t),\lambda(t))\right) \equiv 0, \tag{17}$$

for all $j=0,\dots,(p_k+p_l)/2-1$, $1 \leq k,l \leq m$, whereas bang-bang components u_l can be substituted by $u_l^{\min}$ and $u_l^{\max}$ respectively. We point out that (17) often gives additional conditions to eliminate the adjoints from the singular control. For further details, we refer e.g. to Krener [25] or the examples in Vossen/Maurer [26] and Chyba/Sussmann/Maurer/Vossen [27].

3.2 Transformation to a Finite-Dimensional Problem

We are going to formulate an optimization problem involving the optimization vector

$$z := (x_0^T, t_1, \dots, t_d, t_{d+1})^T \in \mathbb{R}^{n+d+1}, \quad 0 = t_0 < t_1 < \cdots < t_d < t_{d+1} = t_f,$$

and use the following notations:

$$J_i := [t_{i-1}, t_i], \quad i = 1,\dots,d+1, \qquad \theta := \{t_1,\dots,t_d\}.$$

Along the optimal trajectory $\hat{\mathcal{T}}$, we use the notations $\hat{z}$, $\hat{J}_i$ and $\hat{\theta}$, respectively. The functions $u^i(t,x)$ in (15) piecewise define a new function,

$$u(t,x) := u^i(t,x), \quad t \in J_i,\ i=1,\dots,d+1. \tag{18}$$

Let $x(\cdot,z)$ be the absolutely continuous solution of the initial value problem (IVP)

$$x(0)=x_0, \qquad \dot{x}(t)=f(t,x(t),u(t,x(t)))=h(t,x(t)), \quad t\in[0,t_f], \tag{19}$$

where h is piecewise defined as $h(t,x):=h^i(t,x)$ on each interval J_i with

$$h^i(t,x):=f(t,x,u^i(t,x)), \quad i=1,\dots,d+1. \tag{20}$$

The initial value x_0 is taken from the optimization vector z. Obviously, we obtain $x(t,\hat{z})=\hat{x}(t)$. Under Assumptions 3.1–3.3, the optimal control problem can be reformulated as the following $(n+d+1)$-dimensional nonlinear optimization problem, which will be referred to as the *induced optimization problem*:

$$\begin{aligned} \min \quad & G(z):=g(x_0,x(t_f,z),t_f), \\ \text{s.t.} \quad & \Phi(z):=\phi(x_0,x(t_f,z),t_f)=0. \end{aligned} \tag{21}$$

Remark 3.2 The formulation of the induced problem (21) is based on substituting u via the function $u(t,x)$. As the function $z\mapsto u(t,x(t,z))$ is continuous for all t, Assumption 3.2 ensures that the control constraint (4) is fulfilled in a neighborhood of $\hat{z}$ and can hence be omitted in (21).

Remark 3.3 All fixed components of the optimization vector z should be substituted into the functions g and ϕ and eliminated from z. Furthermore, all constraints in the function ϕ including only the fixed components of z are deleted from (21).

The Lagrangian function for problem (21) is given by

$$\mathcal{L}(z,\rho_0,\rho)=\rho_0 G(z)+\rho\Phi(z), \tag{22}$$

with a scalar $\rho_0\ge 0$ and a row vector $\rho\in\mathbb{R}^r$. Obviously,

$$\mathcal{L}(\hat{z},\rho_0,\rho)=l(\hat{x}_b,\hat{t}_f,\rho_0,\rho). \tag{23}$$

The following optimality conditions can be found, e.g., in Fiacco/McCormick [28]. First-order necessary optimality conditions for problem (21) are given by

$$\mathcal{L}_z(\hat{z},\rho_0,\rho)=\rho_0 G_z(\hat{z})+\rho\Phi_z(\hat{z})=0. \tag{24}$$

The optimal vector $\hat{z}$ is called *normal* if the matrix $\Phi_z(\hat{z})$ has maximal rank r. In this case, one can set $\rho_0=1$ and the multiplier ρ is unique. Second-order sufficient optimality conditions for problem (21) in the normal case are given by

$$\begin{aligned} &\text{(a)} \quad \mathcal{L}_z(\hat{z},\rho_0,\rho)=0, \\ &\text{(b)} \quad \operatorname{rank}(\Phi_z(\hat{z}))=r, \\ &\text{(c)} \quad \bar{z}^T\mathcal{L}_{zz}(\hat{z},\rho_0,\rho)\bar{z}>0 \quad \forall\bar{z}\in\operatorname{Ker}(\Phi_z(\hat{z}))\setminus\{0\}. \end{aligned} \tag{25}$$

We note that condition (c) can be verified as described in Fiacco/McCormick [28] and Büskens [18]. Define the $((n+d+1-r)\times(n+d+1-r))$-dimensional *reduced Hessian matrix* H_{red} by

$$H_{\text{red}} := N^T \mathcal{L}_{zz}(\hat{z}, \rho_0, \rho) N \tag{26}$$

where the columns of the $((n+d+1)\times(n+d+1-r))$-matrix N span the kernel of $\Phi_z(\hat{z})$. Then, condition (c) in (25) is equivalent to

$$(\mathrm{c}^*) \quad v^T H_{\text{red}} v > 0 \quad \forall v \in \mathbb{R}^{n+d+1-r} \setminus \{0\}. \tag{27}$$

3.3 Numerical Implementation

Approach (21) is not convenient for numerical computation. We formulate a slightly different induced optimization problem involving the optimization vector

$$\tilde{z} := (x_0^T, \zeta_1, \zeta_2, \ldots, \zeta_d, \zeta_{d+1})^* \in \mathbb{R}^{n+d+1}, \tag{28}$$

where $\zeta_i := t_i - t_{i-1}$, $i = 1, \ldots, d+1$, are the arc durations. This transformation technique was already described by Kaya/Noakes [29] and Maurer et al. [30] for bang-bang controls. A similar approach was also used by Lee et al. [31]. It is easy to see that z and $\tilde{z}$ are related through $\tilde{z} = Rz$ with

$$R = \begin{pmatrix} I_n & 0 \\ 0 & S \end{pmatrix}, \qquad S = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ -1 & 1 & \ddots & \vdots \\ & \ddots & \ddots & 0 \\ 0 & & -1 & 1 \end{pmatrix}, \tag{29}$$

where I_n denotes the identity matrix of dimension n and $S \in \mathbb{R}^{d+1,d+1}$. We also have $t_f = w\tilde{z}$, where $w = (0, \ldots, 0, 1, \ldots, 1, 1) \in \mathbb{R}^{n+d+1}$ is a row vector with n zeros and $d+1$ ones. Therefore, the new induced optimization problem is as follows:

$$\begin{aligned} \min \quad & \tilde{G}(\tilde{z}) := g(x_0, x(w\tilde{z}, R^{-1}\tilde{z}), w\tilde{z}), \\ \text{s.t.} \quad & \tilde{\Phi}(\tilde{z}) := \phi(x_0, x(w\tilde{z}, R^{-1}\tilde{z}), w\tilde{z}) = 0. \end{aligned} \tag{30}$$

We denote the Lagrangian for problem (30) by $\tilde{\mathcal{L}}$ and obtain

$$\Phi_z = \tilde{\Phi}_{\tilde{z}} R, \qquad \mathcal{L}_z = \tilde{\mathcal{L}}_{\tilde{z}} R, \qquad \mathcal{L}_{zz} = R^T \tilde{\mathcal{L}}_{\tilde{z}\tilde{z}} R. \tag{31}$$

It is clear that necessary and sufficient optimality conditions (24), (25) hold in problem (21) if and only if the corresponding optimality conditions hold in problem (30). The approach (30) can conveniently be implemented using the code NUDOCCCS by Büskens [18], which provides the corresponding trajectory and the adjoints. A detailed description of the computational method for bang-bang controls can be found in Maurer et al. [30]. This technique can be adopted directly for bang-singular controls.

3.4 Controls without Feedback Representation

If contrary to Assumption 3.3 the control can only be determined as a function $u^i(t, x, \lambda)$, i.e. depending also on λ, a modified approach is used for switching time optimization. Detailed information can be found in the internal report [14] by the author or in Vossen/Rehbock/Siburian [32]. For controls which cannot be determined as a function $u^i(t, x, \lambda)$, see also [14] or Büskens et al. [33].

4 Variational Derivatives in the Induced Problem

The verification of the optimality conditions (24), respectively, (25) and hence, the calculation of variational derivatives of the Lagrangian function with respect to the optimization vector z requires the calculation of the variational derivatives of the state $x(\cdot, z)$ with respect to z. All variational derivatives are presented in this section. Due to lack of space in this article, detailed proofs are given in an internal report by the author [14].

4.1 Variational Derivatives of the States

4.1.1 First-Order Variational Derivatives

Definition 4.1 The first-order variational derivatives of the states are defined as

$$v^i(t, z) := \frac{\partial x}{\partial (x_0)_i}(t, z), \quad 1 \le i \le n, \tag{32}$$

$$y^i(t, z) := \frac{\partial x}{\partial t_i}(t, z), \quad 1 \le i \le d, \tag{33}$$

$$y^f(t, z) := \frac{\partial x}{\partial t_f}(t, z). \tag{34}$$

Proposition 4.1 *The function $v^i(t, z)$, $1 \le i \le n$, is the solution of the IVP*

$$v^i(0, z) = e_i, \qquad \dot{v}^i(t, z) = h_x(t, x(t, z))v^i(t, z), \tag{35}$$

where e_i is the ith unit vector. The function $y^i(t, z)$, $1 \le i \le d$, satisfies $y^i(t, z) \equiv 0$ on $[0, t_i[$ and, for $t \ge t_i$, it is the solution of the IVP

$$y^i(t_i, z) = -[\dot{x}]^i = -[h]^i, \qquad \dot{y}^i(t, z) = h_x(t, x(t, z))y^i(t, z), \quad t \ge t_i. \tag{36}$$

The function y^f satisfies $y^f(t, z) \equiv 0$ on $[0, t_f[$ and, for $t = t_f$, we obtain

$$y^f(t_f, z) = \dot{x}(t_f, z) = h(t_f, x(t_f, z)). \tag{37}$$

Proof Variation of a switching time t_i changes the solution of the IVP (19) only in the interval $[t_i, t_f]$. Hence, we have $y^i(t,z) \equiv 0$ on $[0, t_i[$. Furthermore,

$$x(t,z) = x(t_i^-, z) + \int_{t_i^+}^{t} h(s, x(s,z))ds, \quad t \geq t_i.$$

is a solution of IVP (19). Differentiating this equation with respect to t_i, we obtain

$$y^i(t,z) = \dot{x}(t_i^-, z) - \dot{x}(t_i^+, z) + \int_{t_i^+}^{t} h_x(s, x(s,z)) y^i(s,z)\, ds \tag{38}$$

which yields (36). Further details are given in [14]. □

4.1.2 Second-Order Variational Derivatives

Definition 4.2 The second-order variational derivatives of the states are

$$v^{ij}(t,z) := \frac{\partial^2 x}{\partial(x_0)_j \partial(x_0)_i}(t,z) = \frac{\partial v^i}{\partial(x_0)_j}(t,z), \quad 1 \leq i \leq j \leq d, \tag{39}$$

$$w^{ij}(t,z) := \frac{\partial^2 x}{\partial t_j \partial(x_0)_i}(t,z) = \frac{\partial v^i}{\partial t_j}(t,z), \quad 1 \leq i \leq n,\ 1 \leq j \leq d, \tag{40}$$

$$v^{if}(t,z) := \frac{\partial^2 x}{\partial t_f \partial(x_0)_i}(t,z) = \frac{\partial v^i}{\partial t_f}(t,z), \quad 1 \leq i \leq n, \tag{41}$$

$$y^{ij}(t,z) := \frac{\partial^2 x}{\partial t_j \partial t_i}(t,z) = \frac{\partial y^i}{\partial t_j}(t,z), \quad 1 \leq i \leq j \leq d, \tag{42}$$

$$y^{if}(t,z) := \frac{\partial^2 x}{\partial t_f \partial t_i}(t,z) = \frac{\partial y^i}{\partial t_f}(t,z), \quad 1 \leq i \leq d, \tag{43}$$

$$y^{ff}(t,z) := \frac{\partial^2 x}{\partial t_f \partial t_f}(t,z) = \frac{\partial y^f}{\partial t_f}(t,z). \tag{44}$$

Note that we calculate only the entries $\partial^2 x/(\partial z_j \partial z_i)$ for $i \leq j$ as the matrices $\partial^2(x_l)/\partial z^2$ are symmetric for $l = 1, \ldots, n$. Also, the second-order variational derivatives can be computed via certain IVPs. For notational convenience, we omit all arguments of the variations in the ODEs.

Proposition 4.2 *The second-order variational derivatives satisfy*

$$1 \leq i \leq j \leq d: \quad v^{ij}(0,z) = 0, \qquad \dot{v}^{ij} = h_x v^{ij} + (v^i)^T h_{xx} v^j \tag{45}$$

$$\begin{aligned} 1 \leq i \leq n,\ 1 \leq j \leq d: \quad & w^{ij}(t_j, z) = -[h_x]^j v^i(t_j, z), \\ & \dot{w}^{ij} = h_x w^{ij} + (v^i)^T h_{xx} y^j \end{aligned} \tag{46}$$

$$1 \le i \le n: \quad v^{if}(t_f, z) = \dot{v}^i(t_f, z) = h_x(t_f, x(t_f, z))v^i(t_f, z) \tag{47}$$

$$\begin{aligned} 1 \le i \le d: \quad & y^{ii}(t_i, z) = -[h_t]^i - [h_x]^i h^{i-} - h_x^{i+} y^i(t_i, z) \\ & \dot{y}^{ii} = h_x y^{ii} + (y^i)^T h_{xx} y^i \end{aligned} \tag{48}$$

$$\begin{aligned} 1 \le i < j \le d: \quad & y^{ij}(t_j, z) = -[h_x]^j y^i(t_j, z), \\ & \dot{y}^{ij} = h_x y^{ij} + (y^i)^T h_{xx} y^j \end{aligned} \tag{49}$$

$$1 \le i \le d: \quad y^{if}(t_f, z) = h_x(t_f, x(t_f, z))y^i(t_f, z) \tag{50}$$

Here, $\mu^T h_{xx} \nu$ is a column vector with components $\mu^T (h_k)_{xx} \nu$, $k = 1, \dots, n$. Furthermore, we obtain

$$y^{ff}(t_f, z) = \dot{h}(t_f, x(t_f, z)) = h_t(t_f, x(t_f, z)) + h_x(t_f, x(t_f, z))h(t_f, x(t_f, z)). \tag{51}$$

4.2 Variational Derivatives of the Lagrangian

Consider a trajectory $\hat{\mathcal{T}} = (\hat{x}, \hat{u})$ which satisfies the necessary optimality conditions (7)–(12) of the minimum principle. We use the abbreviations $\hat{v}^i(t) := v^i(t, \hat{z})$, $\hat{y}^i(t) := y^i(t, \hat{z})$ and so on.

4.2.1 First-Order Variational Derivatives

We now calculate explicit representations for the first-order variational derivatives of the Lagrangian with respect to the optimization vector z. A proof for (52) is given. All other proofs can be found in [14].

Proposition 4.3 *The following holds*:

$$\frac{\partial}{\partial (x_0)_i} \mathcal{L}(\hat{z}, \rho_0, \rho) = 0, \quad i = 1, \dots, n, \tag{52}$$

$$\frac{\partial}{\partial t_i} \mathcal{L}(\hat{z}, \rho_0, \rho) = 0, \quad i = 1, \dots, d. \tag{53}$$

If the final time t_f is free, we have

$$\frac{\partial}{\partial t_f} \mathcal{L}(\hat{z}, \rho_0, \rho) = 0. \tag{54}$$

Proof Applying the chain rule and using (23) as well as the transversality conditions (8) and (9), the first-order variational derivatives of the Lagrangian with respect to the free initial values $(x_0)_i$ of the states are given by

$$\begin{aligned} \frac{\partial}{\partial (x_0)_i} \mathcal{L}(\hat{z}, \rho_0, \rho) &= l_{(x_0)_i}(\hat{x}_b, \hat{t}_f, \rho_0, \rho) + l_{x_f}(\hat{x}_b, \hat{t}_f, \rho_0, \rho)\hat{v}^i(\hat{t}_f) \\ &= -\lambda_i(0) + \lambda(\hat{t}_f)\hat{v}^i(\hat{t}_f). \end{aligned} \tag{55}$$

Together with (35), the last term can be written as

$$\lambda_i(0) + \int_0^{\hat{t}_f} \frac{d}{dt}(\lambda \hat{v}^i)\, dt. \tag{56}$$

Let us transform the integrand. We first observe that

$$\lambda h_x = \lambda(f_x + f_u u_x) = (\lambda f)_x + (\lambda f)_u u_x = H_x + H_u u_x = H_x$$

where $H_u u_x = 0$ holds since for each component $1 \le k \le n$, $H_{u_k} = 0$ on singular arcs and $(u_k)_x = 0$ on bang-bang arcs [14]. In view of (7) and (35), we obtain

$$\frac{d}{dt}(\lambda \hat{v}^i) = \dot{\lambda}\hat{v}^i + \lambda\dot{\hat{v}}^i = (-H_x + \lambda h_x)\hat{v}^i = 0. \tag{57}$$

Substituting (56) and (57) into (55) yields (52). □

Lemma 4.1 *Let $\hat{\mathcal{T}} = (\hat{x}, \hat{u})$ be a trajectory which satisfies the necessary conditions* (7)–(12) *of the minimum principle. Then, the first-order variational derivatives of the Lagrangian vanish, i.e.*,

$$\frac{\partial}{\partial z}\mathcal{L}(\hat{z}, \rho_0, \rho) = 0.$$

Corollary 4.1 *Let $\hat{\mathcal{T}} = (\hat{x}, \hat{u})$ be a trajectory which satisfies the necessary conditions* (7)–(12) *of the minimum principle. Then, the necessary conditions* (24) *in the induced optimization problem* (21) *are fulfilled.*

4.2.2 Second-Order Variational Derivatives

We now present explicit representations for the second-order variational derivatives of the Lagrangian with respect to the optimization vector z. Due to the symmetry of the matrix $\mathcal{L}_{zz}$, we investigate only the derivatives $\mathcal{L}_{z_i z_j}$ for $i \le j$. For notational convenience, we drop all arguments in the endpoint Lagrangian l and its partial derivatives which are evaluated at $(\hat{x}_b, \hat{t}_f, \rho_0, \rho)$ as well as the argument $(\hat{z}, \rho_0, \rho)$ of the function $\mathcal{L}$. Proofs are given in [14].

Proposition 4.4 *For $1 \le i \le j \le n$, we have*

$$\begin{aligned}\frac{\partial^2 \mathcal{L}}{\partial (x_0)_j \partial (x_0)_i} &= l_{(x_0)_i (x_0)_j} + l_{(x_0)_i x_f}\hat{v}^j(\hat{t}_f) + (\hat{v}^i(\hat{t}_f))^T\left(l_{x_f (x_0)_j} + l_{x_f x_f}\hat{v}^j(\hat{t}_f)\right)\\ &\quad + \int_0^{\hat{t}_f} (\hat{v}^i)^T(H_{xx} + H_{xu}u_x + (u_x)^T H_{ux})\hat{v}^j\, dt.\end{aligned} \tag{58}$$

For $i = 1, \ldots, n$ and $j = 1, \ldots, d$, the following holds:

$$\frac{\partial^2 \mathcal{L}}{\partial t_j \partial (x_0)_i} = l_{(x_0)_i x_f}\hat{y}^j(\hat{t}_f) + \hat{v}^i(\hat{t}_f) l_{x_f x_f}\hat{y}^j(\hat{t}_f)$$

$$+\int_{\hat{t}_j}^{\hat{t}_f} (\hat{v}^i)^T (H_{xx} + H_{xu}u_x + (u_x)^T H_{ux})\hat{y}^j dt. \tag{59}$$

For $i = 1, \ldots, n$, we obtain

$$\begin{aligned}\frac{\partial^2 \mathcal{L}}{\partial t_f \partial (x_0)_i} &= l_{(x_0)_i t_f} + l_{(x_0)_i x_f} \hat{y}^f(\hat{t}_f) \\ &\quad + \hat{v}^i(\hat{t}_f)^T \big(l_{x_f t_f} + l_{x_f x_f} \hat{y}^f(\hat{t}_f)\big) + H_x(\hat{t}_f)\hat{v}^i(\hat{t}_f).\end{aligned} \tag{60}$$

For $i = 1, \ldots, d$, we have

$$\begin{aligned}\frac{\partial^2}{\partial t_i \partial t_i}\mathcal{L}(\hat{z}, \rho_0, \rho) &= D^i(H) - [H_x]^i \hat{y}^i(\hat{t}_i) + \hat{y}^i(\hat{t}_f)^T l_{x_f x_f} \hat{y}^i(\hat{t}_f) \\ &\quad + \int_{\hat{t}_i}^{\hat{t}_f} (\hat{y}^i)^T (H_{xx} + H_{xu}u_x + u_x^T H_{ux})\hat{y}^i \, dt.\end{aligned} \tag{61}$$

For $1 \le i < j \le d$, we get

$$\begin{aligned}\frac{\partial^2}{\partial t_j \partial t_i}\mathcal{L}(\hat{z}, \rho_0, \rho) &= -[H_x]^j \hat{y}^i(\hat{t}_j) + \hat{y}^j(\hat{t}_f)^T l_{x_f x_f} \hat{y}^i(\hat{t}_f) \\ &\quad + \int_{\hat{t}_j}^{\hat{t}_f} (\hat{y}^j)^T (H_{xx} + H_{xu}u_x + u_x^T H_{ux})\hat{y}^i \, dt.\end{aligned} \tag{62}$$

For $i = 1, \ldots, d$, we obtain

$$\frac{\partial^2}{\partial t_f \partial t_i}\mathcal{L}(\hat{z}, \rho_0, \rho) = (\hat{y}^i(\hat{t}_f))^T \big(l_{x_f x_f} \hat{y}^f(\hat{t}_f) + l_{x_f t_f}\big) + (H_x \hat{y}^i)(\hat{t}_f). \tag{63}$$

The following holds:

$$\begin{aligned}\frac{\partial^2}{\partial t_f \partial t_f}\mathcal{L}(\hat{z}, \rho_0, \rho) &= (\hat{y}^f(\hat{t}_f))^T \big(l_{x_f x_f} \hat{y}^f(\hat{t}_f) + l_{x_f t_f}\big) \\ &\quad + l_{t_f x_f} \hat{y}^f(\hat{t}_f) + l_{t_f t_f} + (H_t + H_x f)(\hat{t}_f).\end{aligned} \tag{64}$$

Lemma 4.2 *Let $\hat{\mathcal{T}} = (\hat{x}, \hat{u})$ be a trajectory which satisfies the necessary conditions* (7)–(12) *of the minimum principle. Then, the second-order variational derivatives of the Lagrangian can be computed on the basis of only first-order variational derivatives of the states.*

4.3 Variational Derivatives of the Function Φ

If the induced problem involves constraints, it is essential to compute the variational derivatives of the function Φ for the verification of second-order sufficient conditions (25). They can be obtained as

$$\frac{\partial}{\partial (x_0)_i}\Phi(\hat{z}) = \phi_{(x_0)_i}(\hat{x}_b, \hat{t}_f) + \phi_{x_f}(\hat{x}_b, \hat{t}_f)\hat{v}^i(\hat{t}_f), \quad i = 1, \ldots, n,$$

$$\frac{\partial}{\partial t_i}\Phi(\hat{z}) = \phi_{x_f}(\hat{x}_b, \hat{t}_f)\hat{y}^i(\hat{t}_f), \quad i = 1, \dots, d,$$
$$\frac{\partial}{\partial t_f}\Phi(\hat{z}) = \phi_{x_f}(\hat{x}_b, \hat{t}_f)\hat{y}^f(\hat{t}_f) + \phi_{t_f}(\hat{x}_b, \hat{t}_f). \tag{65}$$

4.4 Main Result

Using Lemma 4.2 and formulas (65), we come to our main result in this section.

Theorem 4.1 *The second-order sufficient conditions* (25) *in the induced optimization problem* (21) *can be verified on the basis of only first-order variational derivatives of the state trajectory.*

We point out that, due to Theorem 4.1, one can dispense with solving the

$$\frac{1}{2}d(d+1)n + dn^2 + \frac{1}{2}d(d+1)n = dn(d+n+1)$$

IVPs (45), (46), (48) and (49) for the second-order variational derivatives of the state trajectory which is a strong simplification and speedup for the numerical verification of second-order sufficient optimality conditions in the induced problem.

To summarize, the procedure of our method is as follows:

Step 1: Find a control structure (see the beginning of Sect. 3).
Step 2: Solve the induced optimization problem and obtain the corresponding trajectory $\hat{\mathcal{T}} = (\hat{x}, \hat{u})$ as well as the adjoint variable λ.
Step 3: Use (35), (36) and (37) to compute $\partial x/\partial z$.
Step 4: Use (58)–(65) to compute L_{zz} and ϕ_z and verify SSC.

5 Numerical Examples

In this section, we illustrate the previously described methods and results with two numerical examples, a slightly changed model of the optimal control of a van der Pol oscillator given by James [34] and the Goddard problem, see Bryson/Ho [15] and Maurer [16]. For convenience, we shall drop all superscripts denoting the optimal solution in the numerical examples.

Step 1 of the procedure described at the end of the Sect. 4 is accomplished as follows. We will discretize the differential equations with the method of Heun, which is of error order 2, see Stoer/Bulirsch [35], and use the code IPOPT to solve the resulting high-dimensional optimization problem. This reveals the control structure as well as approximate values of the switching times which we use as an initial guess for Step 2. For the implementation of Step 2, we choose the code NUDOCCCS. As the time transformation in the induced problem can produce a stiff dynamical system, we use a Runge–Kutta method of error order 7 which is already integrated into the code NUDOCCCS. After the optimization, we use again a Runge–Kutta method of order 7 for solving the initial-value problems to determine the variational derivatives in Steps 3 and 4.

5.1 Van der Pol Oscillator

We consider a van der Pol oscillator problem with fixed final time $t_f = 4$. The control u is scalar.

$$\begin{aligned}
\min \quad & x_3(t_f), \\
\text{s.t.} \quad & \dot{x}_1 = x_2, \\
& \dot{x}_2 = -x_1 + x_2(1 - x_1^2) + u, \\
& \dot{x}_3 = \frac{1}{2}(x_1^2 + x_2^2), \\
& x_1(0) = 0, \qquad x_2(0) = 1, \qquad x_3(0) = 0, \\
& -1 \le u(t) \le 1 \quad \forall t \in [0, t_f].
\end{aligned} \tag{66}$$

The Hamiltonian

$$H(t, x, \lambda, u) = \lambda_1 x_2 + \lambda_2(-x_1 + x_2(1 - x_1^2) + u) + \frac{1}{2}\lambda_3(x_1^2 + x_2^2)$$

leads to the adjoint equations

$$\dot{\lambda}_1 = -x_1 + \lambda_2(1 + 2x_1 x_2), \qquad \dot{\lambda}_2 = -x_2 - \lambda_1 - \lambda_2(1 - x_1^2), \qquad \dot{\lambda}_3 = 0$$

and the transversality conditions $\lambda_1(t_f) = \lambda_2(t_f) = 0$ and $\lambda_3(t_f) = 1$, which yields $\lambda_3 \equiv 1$. The switching function is given by $\sigma(t) = \lambda_2(t)$.

Using the code IPOPT, we find the following control structure with a singular arc in the terminal interval:

$$u(t) = \begin{cases} -1, & 0 \le t \le t_1, \\ 1, & t_1 \le t \le t_2, \\ u^{\text{sing}}(x(t)), & t_2 \le t \le t_f = 4. \end{cases}$$

The singular control on the interval $[t_2, t_f]$ can be obtained as follows. Since the control variable u appears in the second time derivative of the switching function, $\ddot{\sigma} \equiv 0$ reveals an expression $u = u(x, \lambda)$ along a singular arc. The conditions $\sigma = \dot{\sigma} \equiv 0$ can then be used to eliminate λ_1 and λ_2, which yields a feedback expression for the singular control of order $q = 1$:

$$u = u^{\text{sing}}(x) = 2x_1 - x_2(1 - x_1^2).$$

In view of this control structure with two switching times t_1, t_2, the induced optimization problem (21) merely consists in minimizing $x_3(t_f, z)$ with respect to the optimization variable $z = (t_1, t_2) \in \mathbb{R}^2$ respectively, $\tilde{z} = (\xi_1, \xi_2)^T$, $\xi_1 = t_1$, $\xi_2 = t_2 - t_1$. The length of the singular arc is then given by $t_f - \xi_1 - \xi_2$. Note that this is an unconstrained optimization problem as all terminal state values are free. We obtain the

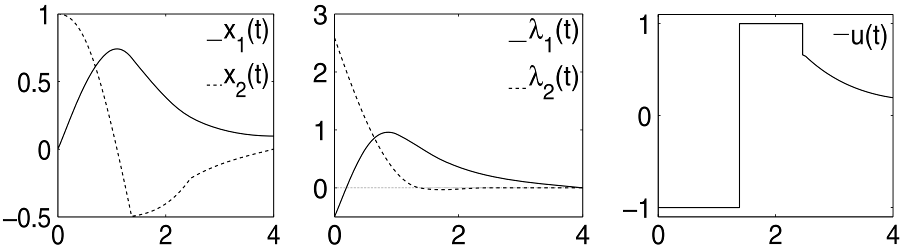

Fig. 1 Optimal states x_1, x_2, adjoints λ_1, λ_2 and optimal control u for the Van der Pol Oscillator

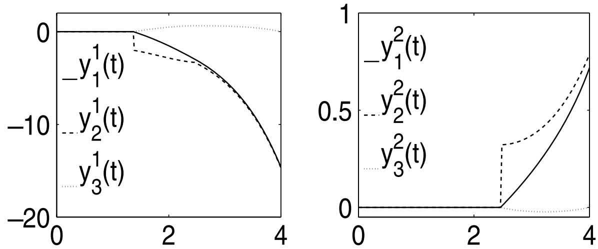

Fig. 2 First-order variational derivatives y^1, y^2 for the Van der Pol Oscillator

representations

$$h^i(x) = \begin{pmatrix} x_2 \\ -x_1 + x_2(1-x_1^2) + (-1)^i \\ \frac{1}{2}(x_1^2 + x_2^2) \end{pmatrix}, \quad i = 1, 2, \qquad h^3(x) = \begin{pmatrix} x_2 \\ x_1 \\ \frac{1}{2}(x_1^2 + x_2^2) \end{pmatrix}$$

and NUDOOCCCS computes the following solution depicted in Fig. 1 with optimal values $t_1 = 1.366733$, $t_2 = 2.460831$ and $x_3(t_f) = 0.7576179$.

Let us now verify the second-order sufficient conditions (25). In a first step, we calculate the variational derivatives. Due to (36), the first-order derivatives can be derived via the IVPs

$$\begin{aligned} y^1(t_1) &= (0, -[u]^1, 0)^T, \qquad \dot{y}^1 = \begin{cases} h_x^2 y^1, & t \in J_2, \\ h_x^3 y^1, & t \in J_3, \end{cases} \\ y^2(t_2) &= (0, -[u]^2, 0)^T, \qquad \dot{y}^2 = h_x^3 y^2, \quad t \in J_3. \end{aligned} \tag{67}$$

Here, the data $[u]^1 = 2$ and $[u]^2 = -0.3233521$ are taken from the solution depicted in Fig. 1. The solution of the IVP (67) is shown in Fig. 2.

Together with (61) and (62), we can now derive the matrix $\mathcal{L}_{zz}$ as

$$\mathcal{L}_{zz}(z, \rho_0, \rho, p_0) = \begin{pmatrix} 215.1022 & -10.5035 \\ -10.5035 & 0.5623 \end{pmatrix}. \tag{68}$$

This matrix is positive definite with eigenvalues 215.615 and 0.0492936 which, in view of the SSC (25), implies that the switching times are optimal since z is normal.

A second method for verifying the SSC is to calculate the values of the Lagrangian function for slightly different values of the switching times and then obtaining the

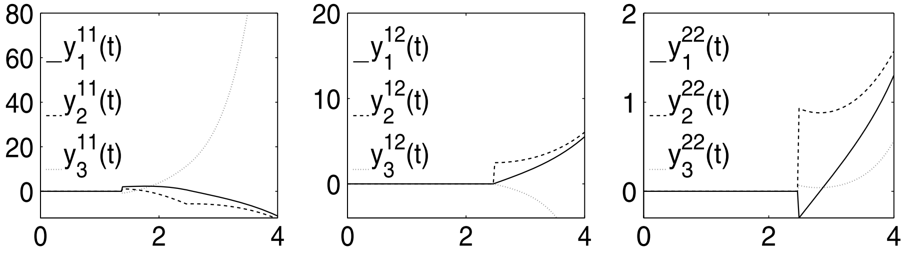

Fig. 3 Second-order variational derivatives y^{11}, y^{12}, y^{22} for the Van der Pol Oscillator

matrix $\mathcal{L}_{zz}$ by numerical differentiation. The code NUDOCCCS accomplishes this method automatically. We note that the Hessian is provided with respect to the optimization vector $\tilde{z}$. However, the matrix $\mathcal{L}_{zz}$ can be computed via formula (31) and we obtain

$$\tilde{\mathcal{L}}_{\tilde{z}\tilde{z}} = \begin{pmatrix} 194.9295 & -9.9704 \\ -9.9704 & 0.5643 \end{pmatrix}, \qquad \mathcal{L}_{zz} = \begin{pmatrix} 215.4346 & -10.5347 \\ -10.5347 & 0.5643 \end{pmatrix}, \tag{69}$$

with eigenvalues 215.95 and 0.0490384 which is very similar to the result in (68). The maximal relative error of the matrix entries in (69) versus those in (68) is 0.36%; the maximal relative error of the eigenvalues is 0.52%.

In this particular problem, it is also possible to verify the SSC by calculating the second-order variational derivatives y^{ij} as the cost functional is given by $x_3(t_f)$ and there are no constraints in the induced problem. Hence, we have

$$\mathcal{L}_{zz} = \begin{pmatrix} y_3^{11}(t_f) & y_3^{12}(t_f) \\ y_3^{12}(t_f) & y_3^{22}(t_f) \end{pmatrix}.$$

Formulas (46) yield the following variational derivatives y^{ij}, which are shown in Fig. 3. From these data, we extract the matrix $\mathcal{L}_{zz}$ with nearly the same values as in (68). Again, the relative errors are smaller than 1%.

Note that Fig. 2 also illustrates that the first-order necessary conditions in the induced problem are fulfilled since $\mathcal{L}_{t_1} = y_3^1(t_f)$ and $\mathcal{L}_{t_2} = y_3^2(t_f)$ vanish.

5.2 Goddard Problem

We present results of switching time optimization for the Goddard problem. This model was introduced in Bryson/Ho [15] and numerically solved with shooting techniques by Maurer [16]. The state variables are the height h, velocity v and mass m. The scalar control is denoted by u and the free final time is t_f. We note that we have taken over the notations from the references as the notations therein are suitable to the meaning of the occuring functions and parameters.

$$\begin{aligned} &\max \quad h(t_f), \\ &\text{s.t.} \quad \dot{h} = v, \qquad \dot{v} = \frac{1}{m}(cu - D(v,h)) - g(h), \qquad \dot{m} = -u, \end{aligned}$$

$$h(0) = h_0, \qquad v(0) = v_0, \qquad m(0) = m_0, \qquad m(t_f) = m_f,$$
$$0 \le u(t) \le u^{\max} \quad \forall t \in [0, t_f]. \tag{70}$$

The drag function $D(v, h)$, the gravity function $g(h)$ and further data can be found in Maurer [16]. Using the solver IPOPT, we obtain the following optimal control structure:

$$u(t) = \begin{cases} u^{\max}, & 0 \le t \le t_1, \\ u^{\text{sing}}(x(t)), & t_1 \le t \le t_2, \\ 0, & t_2 \le t \le t_f, \end{cases}$$

where, as it is shown in Maurer [16], the singular control of order $q = 1$ can be obtained in feedback form. Hence, the induced optimization problem involving the optimization vector $z = (t_1, t_2, t_f)^T$, respectively, $\tilde{z} = (\zeta_1, \zeta_2, \zeta_3)^T$ is given by

$$\begin{aligned} \min \quad & h(t_f, z), \\ \text{s.t.} \quad & m(t_f, z) - m_f = 0. \end{aligned}$$

NUDOCCCS provides a solution with switching times $t_1 = 4.11526$, $t_2 = 46.04061$ and the final time $t_f = 212.90299$, which is consistent with the results in [16]. Finally, we verify the SSC for this solution z. First-order variational derivatives of the states satisfy IVP (36) and (37). The Hessian matrix of the Lagrangian can be computed in view of (61)–(64). Using (65), the reduced Hessian matrix defined in (26) is obtained as

$$H_{\text{red}} = N^T \mathcal{L}_{zz} N = \begin{pmatrix} 74.082672 & -7.378291 \\ -7.378291 & 9.331096 \end{pmatrix},$$

and hence is positive definite on $\mathbb{R}^2$ with eigenvalues 74.9128 and 8.500999. Therefore, the switching times and the final time are optimal due to the SSC (25) and (27).

We conclude with the remark that NUDOCCCS provides the matrices $\tilde{\mathcal{L}}_{\tilde{z}\tilde{z}}$ and $\tilde{\Phi}_{\tilde{z}}$, which lead to similar matrices $\mathcal{L}_{zz}$ and Φ_z by using the formulas (31). The reduced Hessian is obtained as

$$H_{\text{red}} = \begin{pmatrix} 73.2412 & -7.39793 \\ -7.39793 & 9.32778 \end{pmatrix}$$

with eigenvalues 74.0863 and 8.48265. In comparison to our method, the maximal relative difference of the matrix entries is 1.14%, the maximal relative difference of the eigenvalues is 1.10%. We note that a detailed discussion of these results is given in the report [14].

6 Conclusions

In this paper, optimal control problems with the control variable appearing linearly have been studied. The induced optimization problem, a method for directly optimizing the switching times of bang-singular controls, the free initial states and the free final time, was presented. This method can be used for the verification of a certain suboptimality of a trajectory, namely, optimality in the class of all trajectories with the same control structure if the control has finitely many switching times and can be obtained in feedback form along each switching interval.

For the investigation of the first and second-order optimality conditions in the finite–dimensional induced problem, it was essential to derive first and second-order variational derivatives of the state trajectory. It is shown that these derivatives are solutions of certain initial value problems. Corollary 4.1 shows that first-order necessary conditions in the induced problem are fulfilled if the corresponding trajectory satisfies the conditions of the minimum principle. Furthermore, Theorem 4.1 states that the second-order derivatives of the Lagrangian can be computed on the basis of only first-order variational derivatives of the states. This result significantly simplifies the numerical verification of the sufficient optimality conditions in the induced problem. We emphasize that in our method all variational derivatives are computed by using only the data of the reference trajectory and no calculation of any comparison trajectory is necessary. All formal derivatives of the Hamiltonian and endpoint Lagrangian function can be computed a priori.

Our theoretical results have been illustrated with two numerical examples. The induced optimization problem can conveniently be implemented into the routine NUDOCCCS. A comparison of the derivatives computed by our new method to those computed by NUDOCCCS yields similar results with relative differences of 1%.

Although the induced problem for bang-singular controls treats only the optimality of the switching times, the initial states and the final time, it is on the one hand a very useful and fast tool for solving control problems where the control variable appears linearly and on the other hand may be a first step for finding more general optimality conditions similar to those for purely bang-bang controls. Further investigations of the sufficient conditions in the class of all admissable controls are in progress by A. Dmitruk, L. Poggiolini, G. Stefani and the author.

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