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Optimization methods for solving bang-bang control problems with state constraints and the verification of sufficient conditions

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Abstract

We consider bang–bang control problems with state inequality constraints. It is shown that the control problem induces an optimization problem where the optimization vector consists of all switching times of the bang-bang control and junction times with boundary arcs. The induced optimization problem is a generalization of the one studied in [1], [19], [20], [22] for bang–bang controls without state constraints. We develop second order sufficient conditions (SSC) for the state–constrained control problem which require that (1) the SSC for the induced optimization problem are satisfied and (2) additional conditions for the switching function hold at switching and junction times. An optimization algorithm is presented which simultaneously carries out the second–order test. The algorithm is illustrated on a numerical example in cancer chemotherapy.

I. INTRODUCTION

Second–order sufficient optimality conditions (SSC) for bang–bang controls have been derived in Agrachev, Stefani and Zezza [1] on the basis of an induced optimization problem where the control process is optimized with respect to the unknown switching times of the bang–bang control. The equivalence of this type of SSC with a different form of SSC obtained earlier has recently been shown in [19], [20], [22]. Numerical methods for the verification of optimization based SSC have been developed in Maurer et al. [17] using the so–called arc–parametrization method where the arc–lengths of the bang–bang arcs are optimized.

In this paper, we propose an extension of the methods in [17] for solving bang–bang control problems with *state constraints*. The optimization vector in the induced optimization problem is composed by the switching times and exit–time, resp., exit–time (junction times) of boundary arcs. The numerical method is based on the fact that the optimal control can be determined as a feedback expression on both interior and boundary arcs. We present a numerical test of SSC for the induced optimization problem and conjecture that this test leads to SSC for the state–constrained control problem under the additional assumptions (A1)–(A5) on interior and boundary arcs. We discuss a numerical example, the optimal cancer therapy for a two–compartment model [11], which is shown to satisfy the SSC presented in this paper.

II. OPTIMAL BANG-BANG CONTROL PROBLEMS WITH STATE CONSTRAINTS

We consider state-constrained optimal control problems with control appearing linearly. Let $x(t) \in I\!R^n$ denote the state variable and $u(t) \in I\!R$ the control variable at time $t \in [0, t_f]$ where the final time $t_f > 0$ is either fixed or free. For simplicity, the control is assumed to be scalar. The following optimal control problem will be denoted by (OC): determine a measurable control function $u : [0, t_f] \to I\!R$ and a terminal time $t_f > 0$ such that the pair of functions $(x(\cdot), u(\cdot))$ minimizes the cost functional of Mayer type

$$J(x, u, t_f) := g(x(t_f), t_f) \tag{1}$$

subject to the constraints in the interval $[0, t_f]$,

$$\dot{x}(t) = f(x(t), u(t)) = f_0(x(t)) + f_1(x(t))u(t), \tag{2}$$

$$x(0) = x_0, \quad \varphi(x(t_f), t_f) = 0, \tag{3}$$

$$u_{\min} \le u(t) \le u_{\max}, \qquad u_{\min} < u_{\max}\,, \tag{4}$$

and the scalar state inequality constraint

$$S(x(t)) \le 0 \quad \text{for } \ 0 \le t \le t_f\,. \tag{5}$$

The functions $g : I\!R^n \times I\!R \to I\!R$, $f_0, f_1 : I\!R^n \to I\!R^n$, $\varphi : I\!R^n \times I\!R \to I\!R^r$, $0 \le r \le n$, and $S : I\!R^n \to I\!R$ are assumed to be twice continuously differentiable since we intend to derive and verify second order conditions. The state constraint is assumed to be of *order one* [7], [15], i.e., the total time derivative of the function $S(x(t))$ contains the control explicitly,

$$\begin{aligned} S^1(x, u) : &= S_x(x)f(x, u) = S_x(x)f_0(x) + S_x(x)f_1(x)u \\ &=: a(x) + b(x)u, \end{aligned} \tag{6}$$

where $b(x) = S_x(x)f_1(x) \not\equiv 0$. Here and in the sequel, partial derivatives are denoted by subscripts.

An interval $[\tau_1, \tau_2] \subset [0, t_f]$ is called a *boundary arc* if $S(x(t)) \equiv 0$ holds for all $t \in [\tau_1, \tau_2]$. If τ_1 and τ_2 are maximal with this property, then τ_1 is called *entry-time* and τ_2 is called *exit-time* of the boundary arc; τ_1, τ_2 are also called *junction times*. The following assumption is a standard regularity condition for a boundary arc [7], [14], [16].

(A1) On a boundary arc the following condition holds: $b(x(t)) \neq 0 \quad \forall\, t \in [\tau_1, \tau_2]$.

In view of this assumption, we can compute the *boundary control* on a boundary arc from the equation $S^1(x,u) = a(x) + b(x)u = 0$ as the feedback expression

$$u_b(x) = -a(x)/b(x)\,, \quad u(t) = u_b(x(t))\,. \qquad (7)$$

The following assumption will be needed to determine the multiplier associated with the state constraint explicitly.

(A2) The boundary control lies in the interior of the control region:

$$u_{\min} < u(t) = u_b(x(t)) < u_{\max} \quad \forall\, t \in [\tau_1, \tau_2]\ .$$

Assumptions (A1) and (A2) allow us to formulate first order necessary conditions of Pontryagin's minimum principle in a computationally convenient form. We recall from [7], [16] that the Lagrange multiplier associated with the state constraint (5) is a measure that is represented by a function μ of bounded variation. Using (A1) and (A2) it has been shown in [15], [16], [14], [13] that the measure has a Radon–Nikodym derivative η. Hence, we may write the adjoint equation in a differential form. Suppose now that $\bar{u} : [0, t_f] \to [u_{\min}, u_{\max}]$ is an optimal control with corresponding trajectory $\bar{x}$ which satisfy assumptions (A1) and (A2) and for which the state space constraint is not active at the initial and terminal time,

$$S(x(0)) < 0, \quad S(x(t_f)) < 0\,.$$

In the *direct adjoining approach* [7], [16], the augmented Pontryagin or Hamiltonian function is defined by

$$\begin{aligned} H(t,x,u,\lambda,\mu) &= \lambda f(t,x,u) + \eta S(x) \\ &= \lambda f_0(t,x) + \lambda f_1(t,x)u + \eta S(x)\,, \end{aligned} \qquad (8)$$

where the adjoint variable $\lambda \in I\!R^n$ is a row vector and η is the multiplier associated with the state constraint. In the sequel, we will use the junction theorem in [15], Corollary 5.2 (ii), where it was shown that the adjoint variables are *continuous* at junction times provided that the state constraint is of *first order* and the control is *discontinuous* at junctions. Note that the discontinuity of the control follows from assumption (A2). Then there exist an absolutely continuous (a.c.) adjoint function $\lambda : [0, t_f] \to I\!R^n$, a piecewise a.c. multiplier function $\eta : [0, t_f] \to I\!R$ and a multiplier $\rho \in I\!R^r$ (row vector) such that the following conditions hold a.e. on $[0, t_f]$:

$$\dot{\lambda}(t) = -H_x(\bar{x}(t), \bar{u}(t), \lambda(t), \eta(t)), \qquad (9)$$

$$\lambda(t_f) = l_x(\bar{x}(t_f), t_f, \rho), \qquad (10)$$

$$H(\bar{x}(t), \bar{u}(t), \lambda(t), \eta(t))|_{t=t_f} + l_t(\bar{x}(t_f), t_f, \rho) = 0, \qquad (11)$$

$$\begin{aligned} &H(\bar{x}(t), \bar{u}(t), \lambda(t), \eta(t)) \\ &= \min\,\{H(\bar{x}(t), u, \lambda(t), \eta(t)) \mid u_{\min} \le u \le u_{\max}\}, \end{aligned} \qquad (12)$$

$$\eta(t) \ge 0\,, \quad \eta(t) = 0 \quad \text{if } S(x(t)) < 0, \qquad (13)$$

where $l(x, t_f, \rho) := (g + \rho\varphi)(x(t_f), t_f)$ is the endpoint Lagrangian function. The factor at u in the Hamiltonian is called the *switching function*

$$\sigma(x,\lambda) := \lambda f_1(x)\,, \quad \sigma(t) = \sigma(x(t), \lambda(t))\,. \qquad (14)$$

On *interior arcs* with $S(x(t)) < 0$ the minimum condition (12) yields the control law

$$u(t) = \left\{ \begin{array}{ll} u_{\min}, & \text{if } \sigma(t) > 0 \\ u_{\max}, & \text{if } \sigma(t) < 0 \end{array} \right\}. \qquad (15)$$

The switching times of the control are zeroes of the switching function. A *singular arc* occurs if the switching function $\sigma(t)$ vanishes on an open interval. In this paper, we do not consider singular arcs and make the following assumption

(A3) On interior arcs the control $u(t)$ is bang-bang and has only finitely many switching times.

For a *boundary arc* $[\tau_1, \tau_2]$ it was assumed in (A2) that the control takes values in the interior of the control set. Hence, the minimum condition (12) yields

$$\sigma(t) = \lambda(t) f_1(x(t)) = 0 \quad \forall\, t \in [\tau_1, \tau_2]. \qquad (16)$$

This relation can be interpreted as the property that a boundary control behaves formally like a singular control, a fact that was exploited in [15] to obtain junction theorems. By differentiating (16) and using the adjoint equation (9) we find the following explicit representation of the multiplier $\eta(t)$; cf. [16], [13],

$$\begin{aligned} \eta(t) = [\, &\lambda(t)(f_1)_x(x(t)) f(x(t), u_b(x(t))) \\ &-\lambda(t) f_x(x(t), u_b(x(t))) f_1(x(t))\,] \,/\, b(x(t)), \end{aligned} \qquad (17)$$

where $u_b(x(t))$ is the boundary control (7).

III. The Induced Optimization Problem and Second Order Sufficient Conditions

Under assumptions (A1)–(A3), the optimal control problem can be transcribed into an optimization problem in the following way. We assume that the structure of the optimal control, i.e., the sequence of finitely many bang-bang and boundary arcs, is known. Let $t_i, i = 1, \ldots, s$, be the switching and junction times which are ordered as

$$0 =: t_0 < t_1 < \ldots < t_i < \ldots < t_s < t_{s+1} := t_f.$$

For simplicity, assume that there exists only a single boundary arc $[\tau_1, \tau_2] = [t_k, t_{k+1}]$ with an index $1 \le k \le s$. Then $[0, t_k)$ and $(t_{k+1}, t_f]$ are the interior arcs. By assumption, in every interval $I_j := [t_{j-1}, t_j]$ there exists a function $u^j(x)$ with the property that the optimal control is given by

$$u(t) = u^j(x(t))\,,\ t_{j-1} \le t \le t_j,\ (j = 1, \ldots, s, s+1). \qquad (18)$$

The interval I_{k+1} then represents the boundary arc. The function $u^j(x)$ is either the constant value of the bang-bang control on interior arcs or the boundary control $u^{k+1}(x) = u_b(x) = -a(x)/b(x)$.

Consider now the the *optimization variable*

$$z := (t_1, \ldots, t_{s+1})^* \in I\!R^{s+1}, \quad t_{s+1} := t_f,$$

resp. $z := (t_1, \ldots, t_s)^* \in I\!R^s$ for fixed final time t_f , where the asterisk denotes the transpose. Denote by $x(t; z)$ the absolutely continuous solution of the ODE system

$$\dot{x}(t) = f(x(t), u^j(x(t))) \quad \text{for} \quad t_{j-1} \le t \le t_j \qquad (19)$$

with initial condition $x(0) = x_0$. Then the control problem (OC) can be reformulated as the following *induced optimization problem* (OP) with equality constraints:

$$\begin{array}{lll} (OP) & \text{Minimize} & G(z) := g(x(t_{s+1}; z), t_{s+1}) \\ & \text{subject to} & \Phi(z) := \varphi(x(t_{s+1}; z), t_{s+1}) = 0\,, \\ & & \mathcal{S}(z) := S(x(t_k; z)) = 0\,. \end{array} \tag{20}$$

The last equation arises from the entry-condition for the boundary arc. We consider the Lagrangian for the induced optimization problem (OP) in normal form,

$$L(z, \rho, \beta) = G(z) + \rho\Phi(z) + \beta\mathcal{S}(z) \tag{21}$$

with multipliers $\rho \in I\!R^r$ (row vector) and $\beta \in I\!R$. First order necessary and second order sufficient conditions (SSC) for (20) are well known in the literature. In the following theorem, we consider control problems with free final time which involve the optimization vector $z \in I\!R^{s+1}$.

THEOREM *3.1:* (*SSC for the optimization problem* (OP)) Let $\bar{z}$ be feasible for the optimization problem (20). Suppose there exist multipliers $\rho \in I\!R^r$ and $\beta \in I\!R$ such the the following three conditions hold:

(a) rank $[\,\Phi_z(\bar{z})\,|\,\mathcal{S}_z(\bar{z})\,] = s + 1$,

(b) $L_z(\bar{z}, \rho, \beta) = 0$,

(c) $v^* L_{zz}(\bar{z}, \rho, \beta)v > 0$ for all $v \in I\!R^{s+1}$, $v \neq 0$, with $\Phi_z(\bar{z})v = 0,\ \mathcal{S}_z(\bar{z})v = 0$.

Then $\bar{z}$ is a strict local minimizer of the optimization problem (OP). $\diamond$

Arguments similar to those in [17], [22] reveal that the first order conditions in part (a) and (b) of Theorem 3.1 are closely related to those in (9)–(11) involving the adjoint function $\lambda(t)$. However, on the boundary, we obtain adjoint variables which correspond to the *indirect adjoining approach* described in [7], [16] where the function $S^1(x, u)$ in (6) is adjoined in the Hamiltonian by a multiplier η^1 which is different from η. The multiplier β in the Lagrangian (21) yields the jump condition $\lambda(\tau_1+) = \lambda(\tau_1-) - \beta S_x(x(\tau_1))$ for the adjoint variable at the entry–time τ_1. Moreover, one can show the relation $\beta = \int_{\tau_1}^{\tau_2} \eta(t)dt > 0$.

For bang-bang control problems without state inequality constraints, Agrachev, Stefani, Zezza [1] and Maurer, Osmolovskii [19], [20], [22] have shown that one further needs the so–called *strict bang-bang property* to obtain SSC for the bang–bang control problem. The following assumption gives an extension of the strict bang-bang property to control problems with state space constraints.

(A4) **(a)** on *interior arcs* with switching times t_i, $i = 1, ..., k-1, k+2, ..., s$, it holds:
$\sigma(t_i) = 0, \quad \dot{\sigma}(t_i)(u(t_i-) - u(t_i+)) > 0,$
$\sigma(t) \neq 0 \quad \text{for } t \neq t_i$.

(b) at the entry-time t_k and exit-time t_{k+1} of the *boundary arc* the following conditions hold:
$\dot{\sigma}(t_k-)(u(t_k-) - u(t_k+)) > 0\,,$
$\dot{\sigma}(t_{k+1}+)(u(t_{k+1}-) - u(t_{k+1}+)) > 0\,.$

Finally, we need the property that the multiplier $\eta(t)$ satisfies the *strict complementarity* condition.

(A5) *Strict complementarity*: $\quad \eta(t) > 0 \quad \forall\, t \in [t_k, t_{k+1}]$.

Note that assumptions (A4) and (A5) have also been used in [12], [13] to construct a local field of extremals near the boundary arc. Now we can state second order sufficient conditions for the state constrained control problem (1)–(5); the proof will be published elsewhere.

THEOREM *3.2:* (*SSC for the state–constrained control problem (OC)*) Let $\bar{u}$ be a feasible control for the control problem (1)–(5) which has finitely many switching and junction times $\bar{t}_i$, $i = 1, \ldots, s$ and let $\bar{x}$ be the corresponding trajectory. Suppose there exists an adjoint function $\lambda : [0, t_f] \rightarrow I\!R^n$ and a multiplier $\rho \in I\!R^r$ such that assumptions (A1)–(A5) hold where the multiplier function $\eta : [0, t_f] \rightarrow I\!R$ is defined by (17). Suppose further that the vector $\bar{z} = (\bar{t}_1, \ldots, \bar{t}_s, \bar{t}_{s+1})^* \in I\!R^{s+1}$, $\bar{t}_{s+1} = t_f$, satisfies the SSC in Theorem 3.1. Then the control $\bar{u}$ provides a strict strong minimum for the control problem (OC). $\diamond$

IV. NUMERICAL METHODS FOR SOLVING THE INDUCED OPTIMIZATION PROBLEM

In this section, we shall extend the *arc–parametrization* method in [8], [17] to solve state-constrained control problems. Instead of directly optimizing the switching and junction times t_j, $j = 1, \ldots, s$, one determines the arc durations

$$\xi_j := t_j - t_{j-1}, \quad j = 1, \ldots, s, s+1, \tag{22}$$

of bang–bang and boundary arcs. Therefore, the optimization variable $z = (t_1, \ldots, t_s, t_{s+1})^*$, $t_{s+1} := t_f$, is replaced by the optimization variable

$$\xi := (\xi_1, \ldots, \xi_s, \xi_{s+1})^* \in I\!R^{s+1}, \quad \xi_j := t_j - t_{j-1}. \tag{23}$$

The variables z and ξ are related by a linear transformation involving the regular $(s+1) \times (s+1)$–matrix R,

$$\xi = R\,z, \quad z = R^{-1}\xi,$$
$$R = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ -1 & 1 & \ddots & \vdots \\ & \ddots & \ddots & 0 \\ 0 & & -1 & 1 \end{pmatrix}. \tag{24}$$

In the arc–parametrization method, the time interval $[t_{j-1}, t_j]$ is mapped to the fixed interval $I_j := \left[\frac{j-1}{s+1}, \frac{j}{s+1}\right]$ by the linear transformation

$$t = a_j + b_j\tau, \quad \tau \in I_j = \left[\frac{j-1}{s+1}, \frac{j}{s+1}\right], \tag{25}$$

where $a_j = t_{j-1} - (j-1)\xi_j$, $b_j = (s+1)\xi_j$. Identifying $x(\tau) \cong x(a_j + b_j\tau) = x(t)$ in the relevant intervals, we obtain the ODE system

$$\dot{x}(\tau) = (s+1)\,\xi_j\, f(x(\tau), u^j(x(\tau))) \quad \text{for} \quad \tau \in I_j\,. \tag{26}$$

The solutions in the intervals I_j are concatenated to define the *continuous* solution $x(t) = x(t;\xi)$ in the normalized interval $[0,1]$. When expressed in the new optimization variable ξ, the optimization problem (OP) in (20) gives the following optimization problem $(\widetilde{OP})$:

$$\begin{array}{ll}\text{Minimize} & \tilde{G}(\xi) := g(x(1;\xi),t_f), \quad t_f = \sum_{j=1}^{s+1} \xi_j, \\ \text{subject to} & \widetilde{\Phi}(\xi) := \varphi(x(1;\xi),t_f) = 0\,, \\ & \widetilde{S}(\xi) := S(x(k/(s+1);\xi)) = 0\,. \end{array} \tag{27}$$

Using the linear transformation (24) it can easily be seen that the SSC for the optimization problems (OP) and $(\widetilde{OP})$ are equivalent; cf. similar arguments in [17].

To solve this optimization problem, we use a suitable adaptation of the control package NUDOCCCS in Büskens [3], [5]. Then we can take advantage of the fact that this routine also provides the Jacobian of the equality constraints and the Hessian of the Lagrangian which are needed in the check of the second order condition in Theorem 3.1.

V. Numerical example: two-compartment model in cancer chemotherapy with a state constraint

Ledzewicz and Schättler [11], [12] considered a two-compartment model in cancer chemotherapy and established the optimality using the methods outlined in [13]. Here, we prove optimality by appling the numerical SSC test in Theorem 3.2 which is conceptually different from the one in [13]. The description of the control model is taken from [11]: "The cell cycle is broken into two compartments of which the first combines the first growth phase G_1 and the synthesis phase S while the second contains the second growth phase G_2 and mitosis M. Let $x_i(t), i = 1,2$, denote the number of cancer cells in the i–compartment at time time t." The control u is the drug treatment which is measured by its cell–killing effect. The control model is to *minimize* the cost functional with *fixed* final time t_f

$$J(x,u) = r_1 x_1(t_f) + r_2 x_2(t_f) + \int_0^{t_f} u(t)dt \tag{28}$$

subject to

$$\begin{array}{l}\dot{x}_1 = -a_1 x_1 + 2(1-u)a_2 x_2, \\ \dot{x}_2 = a_1 x_1 - a_2 x_2, \\ x_1(0) = x_{10}, \quad x_2(0) = x_{20} \\ 0 \le u(t) \le 1 \quad \forall\, t \in [0,t_f]. \end{array} \tag{29}$$

The cost functional (28) can be transformed to a functional (1) of Mayer type by introducing the equation $\dot{x}_3 = u$, $x_3(0) = 0$, which yields

$$J(x,u) = g(x(t_f)) = r_1 x_1(t_f) + r_2 x_2(t_f) + x_3(t_f).$$

In addition, we consider the state constraint of order one

$$S(x(t)) := x_1(t) + x_2(t) - \alpha \le 0, \quad 0 \le t \le t_f, \tag{30}$$

which imposes an upper bound on the total number of tumor cells in both compartments. The first total time derivative (6) of $S(x)$ is given by

$$S^1(x,u) = a_2 x_2 - 2a_2 x_2 u\,.$$

Obviously, assumption (A1) is satisfied since $b(x(t)) = -2a_2x_2(t) \neq 0$ on $[0,t_f]$. The data in (28) and (29) are taken from [11]; the initial values x_{10}, x_{20} are extrapolated from this paper:

$$\begin{array}{l} r_1 = 6.94,\ r_2 = 3.94,\ a_1 = 0.197,\ a_2 = 0.356, \\ x_1(0) = x_{10} = 0.86,\ x_2(0) = x_{20} = 0.55,\ t_f = 10\,. \end{array}$$

The parameter α in the state constraint (30) will be assigned the value $\alpha = 1.7$ for which the state constraint becomes active. The augmented Hamiltionian (8) is given by

$$\begin{array}{rcl} H &=& \lambda_1(-a_1x_1 + 2a_2x_2) + \lambda_2(a_1x_1 - a_2x_2) + \sigma u \\ && +\eta(x_1 + x_2 - \alpha), \end{array} \tag{31}$$

where σ is the *switching function*

$$\sigma = \sigma(x,\lambda) = 1 - 2a_2x_2\lambda_1\,. \tag{32}$$

The adjoint equation (9) and the transversality condition (10) yield

$$\begin{array}{ll} \dot{\lambda}_1 = a_1(\lambda_1 - \lambda_2) - \eta, & \lambda_1(t_f) = r_1\,, \\ \dot{\lambda}_2 = a_2(2(u-1)\lambda_1 + \lambda_2) - \eta, & \lambda_2(t_f) = r_2\,. \end{array} \tag{33}$$

The *boundary control* $u_b(x)$ satisfies the equation $S^1(x,u_b(x)) \equiv 0$ which gives

$$u_b(x) \equiv 1/2\,.$$

Hence, the boundary control lies in the interior of the control set and satisfies assumption (A2). The multiplier η for the state constraint (30) is determined by equation (17):

$$\eta(t) = a_1\lambda_1(t)\left(\frac{x_1(t)}{x_2(t)} + 1\right) - a_2\lambda_1(t) - a_1\lambda_2(t)\,. \tag{34}$$

To determine the structure of the optimal control we first discretize the control problem with 500 gridpoints and apply the program NUDOCCCS of Büskens [3]. Figures 1 and 2 display the state, resp., adjoint variables, Figure 3 depicts the optimal control and the switching function and Figure 4 gives the state constrained function $x_1 + x_2$.

The control has two bang-bang arcs and one *boundary arc*:

$$u(t) = \left\{ \begin{array}{lll} 0, & \text{for} & t \in [0,t_1] \\ u_b(x(t)) = \frac{1}{2}, & \text{for} & t \in [t_1,t_2] \\ 1, & \text{for} & t \in [t_2,t_f] \end{array} \right\}. \tag{35}$$

It can be seen from Figure 3, that the optimal control satisfies assumptions (A3) and (A4) since, in particular, for $k = 1$ in (A4) we have $\dot{\sigma}(t_1-) < 0$ and $\dot{\sigma}(t_2+) < 0$. Moreover, Figure 5 shows that the multiplier η satisfies the strict complementarity condition (A5).

It remains to verify the SSC in Theorem 3.1 for the optimization problem (27). The optimization variable is

$$\xi = (\xi_1, \xi_2), \quad \xi_1 = t_1,\ \xi_2 = t_2 - t_1\,.$$

Then the arc–length of the final time interval is given by

$$t_f - \xi_1 - \xi_2, \quad t_f = 10\,.$$

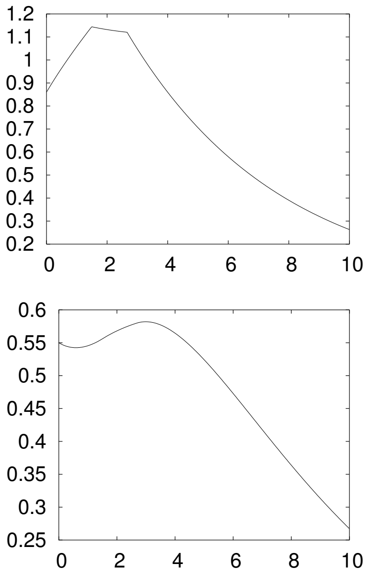

Fig. 1. State variables x_1 and x_2 .

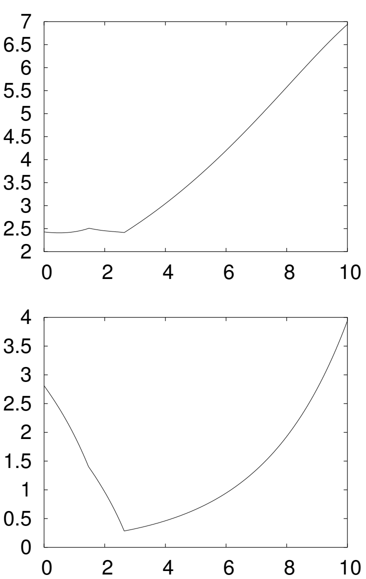

Fig. 2. Adjoint variables λ_1 and λ_2 .

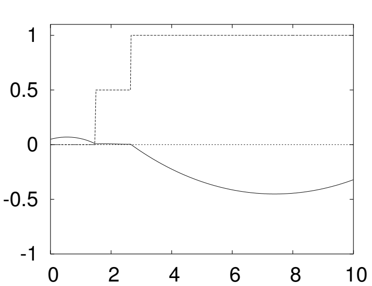

Fig. 3. Optimal control (dotted) and switching function (solid).

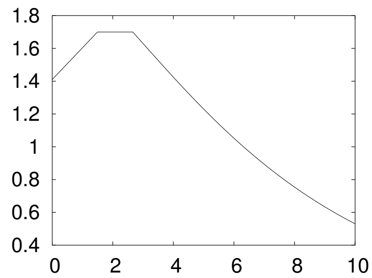

Fig. 4. State constrained function $x_1(t) + x_2(t)$.

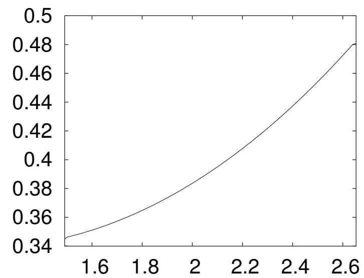

Fig. 5. Multiplier function $\eta(t)$ in (34).

Since no terminal state boundary conditions are prescribed, the only equality constraint is the entry–condition of the boundary arc,

$$x_1(1/3;\xi) + x_2(1/3;\xi) = \alpha = 1.7\,.$$

The code NUDOCCCS gives the following results:

$$\begin{array}{ll} t_1 = \xi_1 = 1.490713, & t_2 = \xi_1 + \xi_2 = 2.653005, \\ \lambda_1(0) = 2.44417, & \lambda_2(0) = 2.82883, \\ x_1(t_f) = 0.2635156, & x_2(t_f) = 0.2673589, \\ J(x,u) = 10.81033\,. & \end{array} \qquad (36)$$

The Hessian of the Lagrangian for (27) is computed as

$$L_{\xi\xi} = \begin{pmatrix} 0.2253187 & 0.1280601 \\ 0.1280601 & 0.0992115 \end{pmatrix}$$

while the Jacobian of the equality constraint is given by

$$\tilde{\mathcal{S}}_\xi = (0.1979670,\ 0).$$

Obviously, the Hessian $L_{\xi\xi}$ is positive definite and we have rank $(\tilde{\mathcal{S}}_\xi) = 1$. Hence, we may conclude that the control (35) referring to the data (36) satisfies the SSC in Theorem 3.1 and provides a strict local minimum of the optimal control problem.

The results on SSC have an immediate application in sensitivity analysis of parametric bang-bang control problems with state constraints. The methods in [10], [17] can be extended to compute parametric sensitivity derivatives of switching and junction times, resp., arclengths of bang–bang and boundary arcs. For the chemotherapy problem under consideration we obtain the following sensitivity derivatives for the arclengths of the first bang-bang arc and the boundary arc:

$$
\begin{aligned}
d\xi_1/da_1 &= -1.513\,, & d\xi_2/da_1 &= 11.99\,,\\
d\xi_1/da_2 &= -3.350\,, & d\xi_2/da_2 &= 0.5165\,,\\
d\xi_1/dx_{10} &= -5.359\,, & d\xi_1/dx_{10} &= 4.421\,,\\
d\xi_1/dx_{20} &= -7.233\,, & d\xi_1/dx_{20} &= 4.077\,.
\end{aligned}
$$

In particular, note the high sensitivity of the arclength of the boundary arc w.r.t. a variation in the parameter a_1 .

VI. Conclusion

We have presented second–order sufficient conditions (SSC) for bang–bang control problems which are subject to a first–order state constraint. The form of these SSC can be regarded as a generalization of those in [1], [19], [20], [22] for purely bang–bang controls. We have discussed numerical methods which efficiently solve the state–constrained bang–bang control problem and provide a test for SSC. The numerical methods were illustrated by an example in cancer chemotherapy. The proposed SSC have been successfully tested on further examples by Altrogge and Goris [2]: (1) a drug displacement problem with a toxicity constraint which was solved in [21]; (2) the control of an image converter with a constraint on the electric field [9]; (3) the control of a nuclear reactor [15]; (4) the cancer chemotherapy for a three–compartment model [23].

The methods in [4], [5], [10], [17] for computing parametric sensitivity derivatives of optimal solutions can be extended to bang–bang control problems with state constraints. In particular, as in [17] one obtains the sensitivity derivatives of switching and junction times which can be used to design real–time control algorithms for the online computation of optimal control and state trajectories under data perturbations; cf., e.g., [6].

References

[1] A.A. Agrachev, G. Stefani and P.L. Zezza, Strong optimality for a bang–bang trajectory, *SIAM J. Control and Optimization*, **41**, (2002), pp. 991–1014.

[2] I. Altrogge, N. Goris, diploma theses, Institut für Numerische Mathematik, Universität Münster, (2004).

[3] C. Büskens, *Optimierungsmethoden und Sensitivitätsanalyse für optimale Steuerprozesse mit Steuer- und Zustands-Beschränkungen*, Dissertation, Institut für Numerische und Angewandte Mathematik, Universität Münster, 1998.

[4] C. Büskens and H. Maurer, Sensitivity analysis and real–time optimization of parametric nonlinear programming problems, in: *Online Optimization of Large Scale Systems*, M. Grötschel et al., eds., Springer–Verlag, Berlin, 2001, pp. 3–16.

[5] C. Büskens and H. Maurer, SQP–methods for solving optimal control problems with control and state constraints: adjoint variables, sensitivity analysis and real–time control, *J. of Computational and Applied Mathematics*, **120**, (2000), pp. 85–108.

[6] C. Büskens and H. Maurer, Nonlinear programming methods for real–time control of an industrial robot, *J. of Optimization Theory and Applications*, **107**, (2000), pp. 505–527.

[7] R.F. Hartl, S.P. Sethi and R.G. Vickson, A survey of the maximum principles for optimal control problems with state constraints, *SIAM Review*, **17**, (1995), pp.181–218.

[8] C.Y. Kaya and J.L. Noakes, Computational method for time-optimal switching control, *J. of Optimization Theory and Applications*, **117**, (2003), pp. 69–92.

[9] J.-H.R. Kim, H. Maurer, Yu. Astrov, M. Bode, and H.G. Purwins, High speed switch–on of a semiconductor gas discharge image converter using optimal control methods, *J. of Computational Physics*, **170**, (2001), pp. 395–414.

[10] J.-H.R. Kim and H. Maurer, Sensitivity analysis of optimal control problems with bang-bang controls, Proc. of the 42nd IEEE Conf. on Decision and Control, Maui, USA, (2003), pp. 3281–3286.

[11] U. Ledzewicz and H. Schättler, Optimal bang–bang controls for a 2–compartment model in cancer chemotherapy, *J. Optimization Theory and Applications*, **114**, (2002), pp. 609–637.

[12] U. Ledzewicz and H. Schättler, Optimal control problems with state space constraints of relative degree 1: Case study of a two–compartment model in cancer chemotherapy, (2004), preprint.

[13] U. Ledzewicz and H. Schättler, A local field of extremals for single–input systems with state space constraints, Proc. of the 43nd IEEE Conf. on Decision and Control, Nassau, The Bahamas, USA, December 2004, pp. 923–928.

[14] K. Malanowski, On normality of Lagrange multipliers for state constrained optimal control problems, *Optimization*, **52**, (2003), pp. 75-91.

[15] H. Maurer, On optimal control problems with bounded state variables and control appearing linearly, *SIAM J. Control and Optimization*, **15**, (1977), pp. 345–362.

[16] H. Maurer, On the minimum principle for optimal control problems with state constraints, Schriftenreihe des Rechenzentrums der Universität Münster, ISSN 0344-0842, (1977).

[17] H. Maurer, C. Büskens, J.-H.R. Kim and C.Y. Kaya, Optimization methods for the verification of second order sufficient conditions for bang–bang controls, *Optimal Control Applications and Methods*, **26**, (2005), pp. 129–156.

[18] H. Maurer, J.-H.R. Kim and G. Vossen, On a state–constrained control problem in optimal production and maintenance, in: C. Deissenberg, R.F. Hartl, eds., *Optimal Control and Dynamic Games, Applications in Finance, Management Science and Economics*, Springer Verlag, (2005), pp. 289–308.

[19] H. Maurer and N.P. Osmolovskii, Quadratic sufficient optimality conditions for bang–bang control problems, *Control and Cybernetics*, **33**, (2003), pp. 555–584.

[20] H. Maurer and N.P. Osmolovskii, Second order sufficient conditions for time–optimal bang–bang control problems, *SIAM J. Control and Optimization*, **42**, (2004), pp. 2239–2263.

[21] H. Maurer and M. Wiegand, Numerical solution of a drug displacement problem with bounded state variables, *Optimal Control Applications and Methods*, **13**, (1992), pp. 43–55.

[22] N.P. Osmolovskii and H. Maurer, Equivalence of second order optimality conditions for bang-bang control problems. Part 1: Main results; Part 2: Proofs, variational derivatives and representations, submitted to *Control and Cybernetics*.

[23] A. Swierniak, U. Ledzewicz and H. Schättler, Optimal control for a class of compartment models in cancer chemotherapy, *Intern. J. of Applied Mathematics and Computer Science*, **13**, (2003), pp. 357–368.