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Solution differentiability for parametric nonlinear control problems with control–state constraints[1)]

by

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Parametric nonlinear control problems subject to mixed control–constraints are considered. The data perturbations are modeled by a parameter p of a Banach space. It is shown that the optimal solution and the adjoint multiplier function are differentiable functions of the parameter p provided that recently developed second–order sufficient optimality conditions (SSC) hold for the unperturbed solution. An elementary proof of solution differentiability is given which is based on ideas from numerical shooting techniques for solving the associated boundary value problem (BVP). The line of proof exploits the close relationships between (1) the variational system corresponding to the BVP, (2) solutions of the associated Riccati ODE and (3) SSC.

Solution differentiability constitutes a theoretical basis for performing a numerical sensitivity analysis. Three non–convex numerical examples are worked out which illustrate the interplay between SSC, shooting techniques and solution differentiability.

Keywords: Parametric control problems, mixed control–state constraints, second–order sufficient conditions, solution differentiability, multipoint boundary value problems, shooting techniques, Riccati equation.

[1)] This paper is an extended version of Maurer and Pesch 1994

1. Introduction

This paper is concerned with sensitivity analysis for parametric nonlinear control problems where the parameter or perturbation p is an element of a Banach space P. The following parametric control problem will be referred to as problem $OC(p)$: minimize the functional

$$J(x,u,p) = g(x(b),p) + \int_a^b L(x(t),u(t),p)dt \tag{1}$$

subject to

$$\dot{x} = f(x(t),u(t),p) \quad \text{for a.e.} \quad t \in [a,b] \; , \tag{2}$$
$$x(a) = \varphi(p) \; , \quad \psi(x(b),p) = 0 \; , \tag{3}$$
$$C(x(t),u(t),p) \le 0 \quad \text{for a.e.} \quad t \in [a,b] \; . \tag{4}$$

We shall not treat the most general case and assume that the control variable u and the inequality constraint (4) are *scalar*. Possible extensions to the vector–valued case will be indicated later. The functions $g : I\!R^n \times P \to I\!R$, $L : I\!R^{n+1} \times P \to I\!R$, $f : I\!R^{n+1} \times P \to I\!R^n$, $\varphi : P \to I\!R^n$, $\psi : I\!R^n \times P \to I\!R^r$, $0 \le r \le n$, and $C : I\!R^{n+1} \times P \to I\!R$ are assumed to be C^2-functions on appropriate open sets. The admissible class is that of piecewise continuous control functions. Later on conditions will be imposed such that the optimal control is continuous and piecewise of class C^1.

Through many papers on sensitivity analysis it has become a well known fact that second order sufficient conditions (SSC) for $OC(p)$ hold fundamental significance for solution differentiability. First, we shall review some theoretical and numerical work done for SSC and solution differentiability. This helps to understand the *main purpose of this paper*: some ideas from numerical shooting techniques for solving $OC(p)$ lead to an elementary and purely finite–dimensional proof of solution differentiability which also integrates recent SSC in a more natural way.

SSC for the unperturbed problem. The problem $OC(p_0)$ corresponding to a fixed parameter $p_0 \in P$ is considered as the *unperturbed* or *nominal* problem. We shall use second order sufficient conditions (SSC) to show that $OC(p_0)$ has a local minimum $x_0(\cdot)$, $u_0(\cdot)$. There are two types of SSC. *Strong* SSC have been deloped in Maurer 1981 and Sorger 1989 for pure state constraints. The results immediately carry over to mixed constraints (4). These strong SSC use a full Riccati equation on $[a,b]$ which does not take into account the active part of the inequality constraints. The *weak* SSC given in Zeidan 1983, Zeidan 1989, Orrell and Zeidan 1988, Pickenhain 1992, Maurer and Pickenhain 1994 and Maurer 1992 aim at deriving SSC under minimal assumptions. The approach consists in constructing a quadratic function which satisfies a Hamilton–Jacobi inequality. The existence of such a function hinges upon the solution of a *modified* Riccati equation which incorporates the tangent space of the active constraints.

Solution differentiability. The nominal solution $x_0(t)$, $u_0(t)$ satisfies a *boundary value problem* (BVP) together with the adjoint function $\lambda_0(t)$. The problem of solution differentiability then consists in finding conditions such that the unperturbed solution $x_0(t)$, $u_0(t)$, $\lambda_0(t)$ can be embedded into a piecewise C^1-family of optimal solutions $x(t,p)$, $u(t,p)$, $\lambda(t,p)$ for the perturbed problem $OC(p)$ with p in a neighborhood of p_0.

Numerical implementation of solution differentiability. Assuming solution differentiability we can approximate the perturbed solution $x(t,p)$, $\lambda(t,p)$ by its first order Taylor–expansion according to

$$x(t,p) \approx x_0(t) + \frac{\partial x}{\partial p}(t,p_0)(p-p_0)\ , \quad \lambda(t,p) \approx \lambda_0(t) + \frac{\partial \lambda}{\partial p}(t,p_0)(p-p_0)\ .$$

The differentials $\partial x(t,p_0)/\partial p$, $\partial \lambda(t,p_0)/\partial p$ are solutions of a *linear* BVP. The numerical data to solve this linear BVP are generated already in the process of computing the unperturbed solution x_0, λ_0. Thus first–order sensitivity calculations are by–products of any solution algorithm for x_0, λ_0. This philosophy has been implemented numerically by a number of authors who, however, do *not* prove that the differentials $\partial x/\partial p$ and $\partial \lambda/\partial p$ actually exist. Control problems without inequality constraints have been treated e.g. by Breakwell, Ho 1965, Breakwell, Speyer, Bryson 1963, Cruz and Perkins 1964, Dorato 1963, Kelley 1962, Kelley 1964, Lee 1965, Lee and Bryson 1989, Pagurek 1965 and Witsenhausen 1965. Inequality constrained problems have been implemented e.g. by Bock 1977, Bock and Krämer–Eis 1981, Krämer–Eis 1985, Kugelmann and Pesch 1990A, Kugelmann, Pesch 1990B and Pesch 1986, Pesch 1989A, Pesch 1989B. These authors use the efficient multiple shooting method for solving BVPs.

The optimization approach for solution differentiability. Sensitivity results for *finite–dimensional* optimization problems are summarized in Fiacco's book, Fiacco 1983. The extensions of these results to optimization problems in *Hilbert–spaces* can be found in Alt 1980, Alt 1989, Alt 1991, Colonius and Kunisch 1991, Dontchev 1983, Ito and Kunisch 1992, Malanowski 1984A – Malanowski 1992, Wiercbicki and Kurcyusz 1977. The Hilbert–space context arises for control problems with control variable appearing *linearly* in the dynamics. The general nonlinear control problem requires the *Banach–space* setting which becomes more complicated due to the so–called *two–norm discrepancy*: compare Dontchev et al. 1992 and Malanowski 1991–Malanowski 1993B for problems with state independent constraints (4).

Solution differentiability via BVP and shooting techniques. Maurer and Pesch 1991–Maurer and Pesch 1994 develop a more *elementary* approach to solution differentiability by studying the close relations between

(1) the boundary value problem $BVP(p)$ associated with the necessary conditions for $OC(p)$,

(2) the corresponding variational system and its Riccati ODE,

(3) SSC for $OC(p)$.

Using shooting techniques for solving $BVP(p)$, solution differentiability proceeds in two steps.

First step. A C^1-family of extremals $x(t,p)$, $\lambda(t,p)$ is constructed which satisfies the parametric $BVP(p)$. Section 2 gives a careful account of the numerical assumptions for setting up $BVP(p)$. Section 3 briefly discusses the shooting method for solving $BVP(p)$ and studies the structure of the Jacobian for the shooting procedure. We will show that a controllability condition and a junction condition at the boundary of the inequality constraint (4) imply the regularity of the Jacobian. Then the implicit function theorem yields the desired C^1-family $x(t,p)$, $\lambda(t,p)$.

Second step. It remains to verify that the constructed family of solutions to $BVP(p)$ is indeed optimal for $OC(p)$. For that purpose, section 4 is devoted to establishing a bridge between $BVP(p)$, its variational system and the weak SSC given in Maurer 1992, Maurer and Pickenhain 1994. When SSC are imposed, solution differentiability is an immediate consequence of the first step. The results are summarized in Theorem 5.1 which provides the basis for sensitivity analysis in section 5 where an inhomogeneous linear BVP for the differentials $\partial x/\partial p$ and $\partial\lambda/\partial p$ is derived.

Numerical examples. There seems to be a considerable deficit of explicit numerical examples for sensitivity analysis. Section 6 present three *non–convex* control problems taken from Maurer and Pesch 1993, Maurer and Pesch 1994 which illustrate the use of SSC. For these examples, all assumptions needed for solution differentiability in Theorem 5.1 will be checked explicitly.

2. The parametric boundary value problem for $OC(p)$

The reader is assumed to have some basic knowledge on necessary optimality conditions for control problems with inequality constraints; compare e.g. Neustadt 1976. The Hamiltonian for the unconstrained problem (1)–(3) is

$$H(x,u,\lambda,p) = L(x,u,p) + \lambda^* f(x,u,p), \quad \lambda \in I\!R^n\,, \tag{5}$$

whereas the *augmented* Hamiltonian for the constrained problem $OC(p)$ is defined by

$$\tilde{H}(x,u,\lambda,\mu,p) = H(x,u,\lambda,p) + \mu C(x,u,p), \quad \mu \in I\!R\,. \tag{6}$$

The adjoint function $\lambda : [a,b] \to I\!R^n$ and the multiplier function $\mu : [a,b] \to I\!R$ with

$$\mu(t) \geq 0 \quad \text{and} \quad \mu(t)C(x(t),u(t),p) = 0 \text{ on } [a,b]\,, \tag{7}$$

are determined by a suitable boundary value problem (BVP). Before setting up an appropriate form of such a BVP we shall introduce some more assumptions on

- the structure of the unperturbed solution (x_0, u_0),
- the regularity of the Hamiltonian H along interior arcs,
- the regularity of the constraint (4) along boundary arcs,
- junctions of interior arcs and boundary arcs.

The following assumptions have become standard in the numerical analysis of problem $OC(p)$ with a regular Hamiltonian although such assumptions are not always stated clearly.

The structure of the unperturbed solution (x_0, u_0).

The *active set* or boundary part of the inequality constraint $C(x,u,p_0) \leq 0$ is supposed to consist of $r \geq 1$ *boundary arcs*, i.e. we have

$$\{t \in [a,b] \mid C(x_0(t),u_0(t),p_0) = 0\} = \bigcup_{i=1}^{r} [t^0_{2i-1}, t^0_{2i}] \tag{8}$$

with $t^0_{2i-1} < t^0_{2i}$. It suffices to consider the case $r = 1$ and for simplicity we also assume $a < t^0_1 < t^0_2 < b$. The points t^0_1, t^0_2 are called *junction points* with the boundary arc. The case that the active set may also contain isolated points τ_i (*contact points*) will not be considered here. Contact points are spurious under the assumptions introduced below and hence are not stable with respect to perturbations. From (8) we can expect that the perturbed solution $x(t,p)$, $u(t,p)$ has one boundary arc for $t_1(p) \leq t \leq t_2(p)$ with $t_i(p_0) = t^0_i$, $i = 1,2$. It will be shown that the junction points $t_1(p)$, $t_2(p)$ are C^1-functions of the parameter p.

C^1-regularity of the Hamiltonian on interior arcs.

Let $\lambda_0 : [a,b] \to I\!R^n$ be the adjoint function associated with (x_0, u_0). This will be a solution of the unperturbed BVP (17) - (20) to be defined below. The following assumption guarantees that the control is a C^1-function on interior arcs.

(A1) (a) **(Strict Legendre–Clebsch condition)**
$H_{uu}(x_0(t),u_0(t),\lambda_0(t),p_0) \geq c > 0$ for $a \leq t \leq t^0_1$ and $t^0_2 \leq t \leq b$.
(b) **(C^1-regularity of the Hamiltonian)**
There exists a uniquely defined C^1-function $u(x,\lambda,p)$ such that
$$u(x,\lambda,p) = arg \min_{u \in I\!R} H(x,u,\lambda,p)$$

holds for all (x, λ, p) in a neighborhood of the trajectory
$x_0(t), \lambda_0(t), p_0$ for $a \le t \le t_1^0$ and $t_2^0 \le t \le b$.

The strict Legendre–Clebsch condition **(A1)(a)** excludes all control problems with control appearing linearly, i.e. bang-bang or singular controls. It should be noted that the C^1-regularity of the Hamiltonian does not follow from part (a). Consider e.g. $L(x,u,p) = (u^2-p)^2$, $f(x,u,p) = u$ and $p_0 = 1$. Here (a) holds but (b) is violated since any control $u(x,p) = \pm\sqrt{p}$ is optimal.

It follows by definition that $u_0(t) = u(x_0(t), \lambda_0(t), p_0)$. The function $u(x,\lambda,p)$ in part (b) can be determined locally by the identity

$$H_u(x, u(x,\lambda,p), \lambda, p) = 0\ . \tag{9}$$

By differentiation we obtain the following partial derivatives in view of assumption (a):

$$u_x = -(H_{uu})^{-1} H_{ux}\ , \quad u_\lambda = -(H_{uu})^{-1} f_u^*\ . \quad u_p = -(H_{uu})^{-1} H_{up}\ . \tag{10}$$

Regularity conditions on boundary arcs.

The following assumption is the counterpart to assumption **(A1)**:

(A2) (a) $C_u(x_0(t), u_0(t), p_0) \neq 0$ for $t_1^0 \le t \le t_2^0$.
(b) The equation $C(x,u,p) = 0$ can be solved for a uniquely defined C^1-function $u = u_b(x,p)$ in a neighborhood of $x_0(t), p_0$ for $t_1^0 \le t \le t_2^0$.

Note that condition (b) is stronger than (a). It excludes cases like $C(x,u,p) = u^2 - p = 0$, $p_0 = 1$ where $u = \pm\sqrt{p}$ is not unique. The function $u_b(x,p)$ is called the *boundary control*. By definition we have $u_0(t) = u_b(x_0(t), p_0)$. Since $C(x, u_b(x,p), p) \equiv 0$ differentiation yields in view of (a)

$$\frac{\partial u_b}{\partial x} = -C_u^{-1} C_x\ , \quad \frac{\partial u_b}{\partial p} = -C_u^{-1} C_p\ , \tag{11}$$

where the arguments on the right side are $(x, u_b(x,p), p)$.

Assumption **(A2)** enables us to compute the multiplier function μ for the augmented Hamiltonian $\tilde{H} = H + \mu C$. On the boundary, the optimal control satisfies the condition

$$\tilde{H}_u = H_u + \mu C_u = 0\ . \tag{12}$$

In terms of the variables x,λ,p the multiplier μ can then be expressed as

$$\mu(x,\lambda,p) = -H_u(x, u_b(x,p), \lambda, p)/C_u(x, u_b(x,p), p)\ . \tag{13}$$

The partial derivatives of μ are found by differentiating (12) and using the partial derivatives in (11):

$$\begin{aligned} \mu_x &= C_u^{-1}(\tilde{H}_{uu} C_u^{-1} C_x - \tilde{H}_{ux})\ , \ \mu_\lambda = -C_u^{-1} f_u^*\ ; \\ \mu_p &= C_u^{-1}(\tilde{H}_{uu} C_u^{-1} C_p - \tilde{H}_{up})\ . \end{aligned} \tag{14}$$

Joining interior and boundary arcs.

It is easy to see that assumptions **(A1)**, **(A2)** imply the continuity of the control at junction points t_1, t_2. This leads to the condition

$$C(x(t_i), u(x(t_i), \lambda(t_i), p), p) = 0 , \quad i = 1, 2 , \tag{15}$$

where $u(x, \lambda, p)$ is the minimizing function in **(A1)(b)**. Furthermore it will be required that the unperturbed solution $x_0(t)$,$u_0(t)$ has a *non-tangential* junction with the boundary:

(A3) $\quad \frac{d}{dt} \; C(x_0(t), u_0(t), p_0)|_{t_i^0} \neq 0 , \quad i = 1, 2 .$

Here the derivative is understood as derivative from the left at t_1^0 and as derivative from the right at t_2^0. It will turn out that this condition is essential for constructing perturbed extremal solutions. Conditions (15) and **(A3)** imply that the multiplier μ in (13) satisfies

$$\mu(t_i) = 0 \quad (i = 1, 2) , \quad \dot{\mu}_0(t_1^0) > 0 , \quad \dot{\mu}_0(t_2^0) < 0 ,$$

where μ_0 denotes the multiplier corresponding to (x_0, u_0).

Transversality condition.

The function ψ defining the boundary condition (3) is supposed to satisfy

(A4) $\quad$ rank $\psi_x(x_0(b), p) = r$.

Then there exists a unique multiplier $\nu \in I\!R^r$ such that

$$\lambda(b) = g_x(x(b), p)^* + \psi_x(x(b), p)^* \nu . \tag{16}$$

Condition (16) is void if the final state $x(b)$ is fixed, i.e. if $x(b) = \psi(p)$ holds with a C^1-function $\psi : P \to I\!R^n$.

Under assumptions **(A1)** and **(A2)** the following *parametric* boundary value problem $BVP(p)$ arises for determining the trajectory $x(t)$, the adjoint function $\lambda(t)$, the junction points t_1. t_2 and the multiplier ν:

ODE

$$\dot{x} = \begin{cases} f(x, u(x, \lambda, p), p) & \text{for} \quad t \notin [t_1, t_2] , \\ f(x, u_b(x, p), p) & \text{for} \quad t \in [t_1, t_2] . \end{cases} \tag{17}$$

$$\dot{\lambda} = \begin{cases} -H_x(x, u(x, \lambda, p), \lambda, p) & \text{for} \quad t \notin [t_1, t_2] , \\ -\tilde{H}_x(x, u_b(x, p), \lambda, \mu(x, \lambda, p), p) & \text{for} \quad t \in [t_1, t_2] , \\ \quad \mu(x, \lambda, p) \quad \text{from} \quad (13) . & \end{cases} \tag{18}$$

Boundary and junction conditions.

$$x(a) = \varphi(p) , \quad \psi(x(b), p) = 0 , \quad \lambda(b) = g_x(x(b), p)^* + \psi_x(x(b), p)^* \nu , \tag{19}$$

$$\tilde{C}(x(t_i), \lambda(t_i), p) = 0 \quad (i = 1, 2) , \quad \tilde{C}(x, \lambda, p) := C(x, u(x, \lambda, p), p) . \tag{20}$$

The differentiability properties of $u(x,\lambda,p)$ and $u_b(x,p)$ imply that any solution $x(t)$ and $\lambda(t)$ of $BVP(p)$ is a C^1-function on $[a,b]$. It should be noted that, in addition, the sign condition $\mu(t) = \mu(x(t),\lambda(t),p) \geq 0$ for $t_1 \leq t \leq t_2$ must be checked for optimal candidates $x(t)$ and $\lambda(t)$.

3. Shooting methods for constructing parametric extremals

The shooting procedure treats the initial value $\lambda(a)$, the multiplier ν and the junction points t_1 and t_2 as an unknown parameter

$$s = (s_\lambda, \nu, t_1, t_2) \in I\!R^{n+2}\ , \quad s_\lambda \in I\!R^n\ ,\ \nu \in I\!R^r\ ,\ t_1, t_2 \in I\!R\ .$$

Let $x(t,s,p)$ and $\lambda(t,s,p)$ denote the solution of ODEs (17) and (18) with initial condition

$$x(a,s,p) = \varphi(p)\ , \quad \lambda(a,s,p) = s_\lambda\ . \tag{21}$$

The solution of $BVP(p)$ is equivalent to solving the $n+r+2$ nonlinear equations

$$F(s,p) := \begin{pmatrix} \psi(x(b,s,p),p) \\ \lambda(b,s,p) - (g + \nu^*\psi)^*_x(x(b,s,p),p) \\ \left(\tilde{C}(x,\lambda,p)|_{(t_i,s,p)}\right)_{i=1,2} \end{pmatrix} = 0 \tag{22}$$

for the shooting parameter s as a function of p near p_0. The function $\tilde{C}$ has been introduced in (20).

The unperturbed solution (x_0,λ_0,ν_0) with $s_0 = (\lambda_0(a),\nu_0,t_1^0,t_2^0)$ satisfies $F(s_0,p_0) = 0$ by definition. The classical implicit function theorem can be applied to the parametric equation (22) if the Jacobian of F with respect to s is regular. Henceforth, the argument b, s_0, p_0 will be abbreviated by $[b]$. It easily follows from elementary properties of parametric ODEs that

$$\frac{\partial x}{\partial t_i}[b] = \phi(b,t_i^0)\{f(x_0(t_i^0),u_0((t_i^0)^-),p_0) - f(x_0(t_i^0),u_0((t_i^0)^+),p_0)\}$$

where $\phi(b,t_i^0)$ is the transition matrix for the linear system $\dot{\phi} = f_x^0(t)\phi$. Since $u_0(t)$ is *continuous* at t_i^0 $(i=1,2)$, we get

$$\frac{\partial x}{\partial(t_1,t_2)}[b] = 0\ .$$

In the same way, the relation $\partial\lambda[b]/\partial(t_1,t_2) = 0$ is obtained. Then the Jacobian of $F(s,p)$ at (s_0,p_0) with respect to s becomes

$$\frac{\partial F}{\partial s}(s_0,p_0) = \begin{pmatrix} M[b] & \vdots & \mathbf{O} & \\ \cdots & \vdots & \cdots\cdots\cdots & \\ & \vdots & \dot{C}(t_1^0) & \mathbf{O} \\ * & \vdots & & \\ & \vdots & * & \dot{C}(t_2^0) \end{pmatrix}, \tag{23}$$

where

$$M[b] = \begin{pmatrix} \psi_x[b]\frac{\partial x}{\partial s_\lambda}[b] & \mathbf{O} \\ \frac{\partial \lambda}{\partial s_\lambda}[b] - \Gamma[b]\frac{\partial x}{\partial s_\lambda}[b] & -\psi_x[b]^* \end{pmatrix}, \tag{24}$$

$$\Gamma[b] = (g + \nu_0^*\psi)_{xx}[b]\,, \quad \dot{C}(t_i^0) = \frac{d}{dt}\tilde{C}(x_0(t),\lambda_0(t),p_0)|_{t_i^0}\,.$$

Hence (23) leads to the statement:

$$\frac{\partial F}{\partial s}(s_0,p_0) \text{ is regular } \Leftrightarrow M[b] \text{ in (24) is regular and } \mathbf{(A3)} \text{ holds}\,. \tag{25}$$

Assuming that one of the equivalent statements in (25) holds, the implicit function theorem yields a differentiable function

$$s: V \to I\!R^{n+r+2}\,, \quad V \subset P \text{ neighborhood of } p_0\,,$$

such that $s(p_0) = s_0$ and $s(p) = (s_\lambda(p), \nu(p), t_1(p), t_2(p))$ satisfies

$$F(s(p),p) \equiv 0 \qquad \text{for all} \quad p \in V\,.$$

Then the functions

$$x(t,p) := x(t,s(p),p)\,, \quad \lambda(t,p) := \lambda(t,s(p),p)$$

are solutions of $BVP(p)$ for all $p \in V$ and $x(t,p_0) = x_0(t)$ and $\lambda(t,p_0) = \lambda_0(t)$ holds for $t \in [a,b]$. These functions are C^1-functions with respect to *both* arguments (t,p). This property is obvious for $t \neq t_i(p)$, $i = 1,2$, but it also holds at $(t_i(p),p)$ which will be shown now.

The derivatives $\partial x/\partial t$ and $\partial\lambda/\partial t$ are continuous at $(t_i(p),p)$ since u is continuous and $\mu(t_i(p)) = 0$ holds. Differentiating the identities

$$x(t_1(p)^-,p) = x(t_1(p)^+,p)\,, \quad \lambda(t_1(p)^-,p) = \lambda(t_1(p)^+,p)$$

we immediately see that $\partial x/\partial p$ and $\partial\lambda/\partial p$ are continuous at $(t_i(p),p)$ since $\partial x/\partial t$ and $\partial\lambda/\partial t$ are continuous.

The preceding ideas can be summarized in the following result on the existence of a C^1-family of solutions of $BVP(p)$.

THEOREM 3.1 *Let (x_0, u_0) be feasible for $OC(p_0)$ and let (x_0, λ_0) solve $BVP(p_0)$ such that assumptions* **(A1)**–**(A3)** *hold. Suppose that the $(n+r)\times(n+r)$ shooting matrix $M[b]$ defined in (24) is regular.*

Then there exists a neighborhood $V \subset P$ of p_0 and C^1-functions

$$x, \lambda : [a,b] \times V \to I\!R^n \ , \quad \nu : V \to I\!R^r \ , \quad t_i : V \to I\!R \quad (i = 1,2)$$

such that

(1) $x(t,p_0) = x_0(t)$, $\lambda(t,p_0) = \lambda_0(t)$ *for* $t \in [a,b]$, $\nu(p_0) = \nu_0$ *and* $t_i(p_0) = t_i^0$ $(i = 1,2)$,

(2) $x(\,\cdot\,,p)$, $\lambda(\,\cdot\,,p)$, $\nu(p)$, *and* $t_1(p)$, $t_2(p)$ *are solutions of $BVP(p)$ for every $p \in V$.*

The associated control $u(t,p)$ is defined via **(A1)** and **(A2)** by

$$u(t,p) := \begin{cases} u(x(t,p), \lambda(t,p), p) & \text{for} \quad t \notin [t_1(p), t_2(p)] \\ u_b(x(t,p), p) & \text{for} \quad t \in [t_1(p), t_2(p)] \end{cases} \tag{26}$$

This control is only piecewise a C^1-function and the partial derivatives u_t and u_p are *not* continuous at $(t_i(p), p)$ due to the non–tangential junction in **(A3)**. The multiplier $\mu(t,p)$ on boundary arcs becomes

$$\mu(t,p) := \mu(x(t,p), \lambda(t,p), p) \ , \quad t_1(p) \le t \le t_2(p) \tag{27}$$

with μ from (13).

The next two sections will be devoted to the problem of establishing conditions for the optimality of the pair $(x(t,p), u(t,p))$.

4. The variational system, Riccati ODE and second order sufficient conditions

Second order sufficient conditions (SSC) in a weak form have recently been derived in Maurer 1992, Maurer and Pickenhain 1994, Orrell and Zeidan 1988, Pickenhain 1992, Zeidan 1989. We shall follow the presentation in Maurer 1992 and establish the connection between SSC and the variational system associated with ODEs (17) and (18). In the following, all terms with an upper or lower index zero are evaluated at the unperturbed trajectory x_0, u_0, λ_0, p_0. The notation y and η is used for n-vectors or $n\times n$-matrices which can be interpreted as variational quantities associated with x and λ. The variational system for (17) and (18) at $p = p_0$ is composed by $2n$ linear ODE

$$\dot{y} = A^0(t)y + B^0(t)\eta \ , \quad \dot{\eta} = W^0(t)y - A^0(t)^*\eta \ . \tag{28}$$

On *interior arcs* $t \notin [t_1^0, t_2^0]$ the $n \times n$-matrices herein are given by

$$\left.\begin{array}{rcl} A^0(t) &=& \left(\frac{d}{dx} f(x, u(x,\lambda,p), p)\right)^0 = f_x^0 - f_u^0 (H_{uu}^0)^{-1} H_{ux}^0 \quad , \\ B^0(t) &=& \left(\frac{d}{d\lambda} f(x, u(x,\lambda,p), p)\right)^0 = -f_u^0 (H_{uu}^0)^{-1} (f_u^0)^* \quad , \\ W^0(t) &=& -\left(\frac{d}{dx} H_x(x, u(x,\lambda,p), \lambda, p)\right)^0 \\ &=& -H_{xx}^0 + H_{xu}^0 (H_{uu}^0)^{-1} H_{ux}^0 \quad . \end{array}\right\} \quad (29)$$

These expressions make use of the derivatives u_x and u_λ from (10).

On the *boundary arc* $t \in [t_1^0, t_2^0]$ the matrices are

$$\left.\begin{array}{rcl} A^0(t) &=& \left(\frac{d}{dx} f(x, u_b(x,p), p)\right)^0 = f_x^0 - f_u^0 (C_u^0)^{-1} C_x^0 \quad , \\ B^0(t) &=& \left(\frac{d}{d\lambda} f(x, u_b(x,p), p)\right)^0 = 0 \quad , \\ W^0(t) &=& -\left(\frac{d}{dx} \tilde{H}_x(x, u_b(x,p), \lambda, \mu(x,\lambda,p), p)\right)^0 \\ &=& -\tilde{H}_{xx}^0 + \tilde{H}_{xu}^0 (C_u^0)^{-1} C_x^0 \\ && +(C_x^0)^* (C_u^0)^{-1} (\tilde{H}_{ux}^0 - \tilde{H}_{uu}^0 (C_u^0)^{-1} C_x^0) \quad . \end{array}\right\} \quad (30)$$

These formulae employ the derivatives in (14) and can be found in Pesch 1989A, formula (58); a more detailed derivation is given in Maurer 1992.

Consider now the matrix solution $y(t)$ and $\eta(t)$ of the variational system (28) with initial conditions $y(a) = O_n$ and $\eta(a) = I_n$. By inspecting the shooting procedure (21), (22) it readily follows that

$$y(b) = \frac{\partial x}{\partial s_\lambda}[b] \, , \quad \eta(b) = \frac{\partial \lambda}{\partial s_\lambda}[b] \, .$$

Recall that the regularity of the matrix $M[b]$ in (24) was the main assumption for Theorem 3.1. A numerical check of the regularity of $M[b]$ is provided by the multiple shooting code in Oberle and Grimm 1989.

Next we turn our attention to a matrix Riccati ODE associated to the variational system (28). Following Reid 1972, Chapter III, we consider a symmetric $n \times n$-matrix $Q(t)$ which satisfies the Riccati equation

$$\dot{Q} = -QA^0(t) - A^0(t)^* Q - QB^0(t) Q + W^0(t) \, . \quad (31)$$

Along interior arcs $t \notin [t_1^0, t_2^0]$ this can be rewritten using (29) as

$$\dot{Q} = -Qf_x^0 - (f_x^0)^* Q - H_{xx}^0 + (H_{xu}^0 + Qf_u^0)(H_{uu}^0)^{-1}(H_{ux}^0 + (f_u^0)^* Q). \quad (32)$$

On the boundary arc $t \in [t_1^0, t_2^0]$ the Riccati ODE (31) reduces to a *linear* ODE

$$\dot{Q} = -QA^0(t) - A^0(t)^* Q + W^0(t) \, . \quad (33)$$

Solutions of the Riccati *ODE* (31) are directly related to the follwing weak form of SSC which can be found in Theorem 5.2 of Maurer and Pickenhain 1994.

THEOREM 4.1 (Second–order sufficient conditions) *Let* (x_0, u_0) *be feasible for* $OC(p_0)$. *Assume that there exists an absolutely continuous function* $\lambda_0 : [a,b] \to I\!R^n$ *and a multiplier* $\nu_0 \in I\!R^r$ *such that*

(a) **(A1)** *and* **(A2)** *hold for* $p = p_0$,

(b) (x_0, λ_0, ν_0) *is a solution of* $BVP(p_0)$.*with* $\mu_0(t) \geq 0$ *for* $t_1^0 \leq t \leq t_2^0$ *where the multiplier* μ_0 *is defined by (13),*

(c) the Riccati ODE (31) has a finite symmetric solution Q *in* $[a,b]$ *satisfying the boundary condition*

$$y^*((g + \nu_0^* \psi)_{xx}[b] - Q(b))y \geq 0 \quad \text{for } y \in I\!R^m \text{ with } \psi_x[b]y = 0 \,. \qquad (34)$$

Then (x_0, u_0) *provides a local minimum for* $OC(p_0)$. *Moreover,* $u_0(t)$ *is continuous and is a* C^1*-function for* $t \neq t_i^0 \quad (i = 1, 2)$ *while* x_0 *and* λ_0 *are* C^1*-functions on* $[a,b]$.

5. Solution differentiability and sensitivity analysis

The last two section have prepared all ingredients for conditions establishing solution differentiability. Combining Theorem 3.1 on the existence of perturbed extremals with Theorem 4.2 we arrive at the main result of this paper.

THEOREM 5.1 (Solution differentiability) *Let* (x_0, u_0) *be feasible for* $OC(p_0)$ *with the boundary structure (8). Let* (x_0, λ_0) *be a solution of* $BVP(p_0)$ *such that the following assumptions hold:*

(a) **(A1)**–**(A4)** *are satisfied,*

(b) the multiplier μ_0 *in (13) satisfies the strict complementarity condition* $\mu_0(t) > 0$ *for* $t_1^0 < t < t_2^0$,

(c) the Riccati ODE (31) has a finite symmetric solution Q *on* $[a,b]$ *with boundary conditions (34),*

(d) the matrix $M[b]$ *in (24) is regular.*

Then there exist a neighborhood $V \subset P$ *of* $p = p_0$ *and* C^1*-functions*

$$x, \lambda : [a,b] \times V \to I\!R^n \,, \quad \nu : V \to I\!R^r \,, \quad t_i : V \to I\!R \quad (i = 1, 2)$$

and a function

$$u : [a,b] \times V \to I\!R$$

which is of class C^1 *for* $t \neq t_i(p) \;\; (i = 1, 2)$, *such that the following statements hold:*

(1) $x(t, p_0) = x_0(t)$, $\lambda(t, p_0) = \lambda_0(t)$, $u(t, p_0) = u_0(t)$ *for* $t \in [a,b]$, $\nu(p_0) = \nu_0$ *and* $t_i(p_0) = t_i^0 \;\; (i = 1, 2)$,

(2) the triple $x(\,\cdot\,, p)$, $\lambda(\,\cdot\,, p)$, $u(\,\cdot\,, p)$ *and the multiplier* $\nu(p)$ *satisfies the second-order sufficient conditions in Theorem 4.2 for every* $p \in V$ *and hence the pair* $x(\,\cdot\,, p), u(\,\cdot\,, p)$ *provides a local minimum for* $OC(p)$.

PROOF. Theorem 3.1 yields C^1-functions

$$x, \lambda : [a,b] \times V \to I\!R^n \,, \quad \nu : V \to I\!R^r \,, \quad t_i : V \to I\!R \quad (i = 1, 2)$$

in a neighborhood V of p_0 such that $x(\,\cdot\,,p)$, $\lambda(\,\cdot\,,p)$, $\nu(p)$ and $t_1(p), t_2(p)$ solve $BVP(p)$ for $p \in V$. The associated control $u : [a,b] \times V \to I\!R$ is defined by (26). It remains to verify that the triple $x(\,\cdot\,,p)$, $\lambda(\,\cdot\,,p)$, $u(\,\cdot\,,p)$ is optimal.

We can choose V small enough such that the following two statements are true for $p \in V$:

(a) $H_{uu}(x(t,p), u(t,p), \lambda(t,p), p) \geq c > 0$ for $t \notin [t_1(p), t_2(p)]$.

(b) The Riccati ODE
$\dot{Q} = -QA(t,p) - A(t,p)^*Q - QB(t,p)Q + W(t,p)$
has a finite symmetric solution $Q(\,\cdot\,,p)$ on $[a,b]$ satisfying the boundary conditions (34). The matrices $A(t,p)$, $B(t,p)$ and $W(t,p)$ denote the matrices in (29) for $t \notin [t_1(p), t_2(p)]$ and in (30) for $t \in [t_1(p), t_2(p)]$ evaluated at $x(t,p)$ and $\lambda(t,p)$.

The last statement (b) is a consequence of the continuous dependence of solutions of ODEs on parameters.

Finally, to complete the proof we have to check the sign condition (7) for the C^1-multiplier μ defined in (13) resp. (27):

$$\mu(t,p) = -H_u/C_u \geq 0 \qquad \text{for} \quad t_1(p) \leq t \leq t_2(p).$$

This sign condition follows readily from property (16) and the assumed strict complementary of the unpertubed multiplier μ_0:

$$\dot{\mu}_0(t_1^0) > 0\ ,\ \ \dot{\mu}_0(t_2^0) < 0\ ,\ \ \mu_0(t) > 0 \quad \text{for} \quad t_1^0 < t < t_2^0$$

Hence the pair $(x(\,\cdot\,,p), u(\,\cdot\,,p))$ is indeed optimal for $OC(p)$. ■

The solution differentiability provides a theoretical basis for performing a *sensitivity analysis* where the perturbed solution is approximated by a first order Taylor expansion according to

$$x(t,p) \approx x_0(t) + \frac{\partial x}{\partial p}(t,p_0)(p-p_0)\ ,\ \ \lambda(t,p) \approx \lambda_0(t) + \frac{\partial \lambda}{\partial p}(t,p_0)(p-p_0)\ .$$

The sensitivity differentials

$$y(t) := \frac{\partial x}{\partial p}(t,p_0)\ ,\ \ \eta(t) := \frac{\partial \lambda}{\partial p}(t,p_0)\ ,\quad \nu_p = \frac{d\nu}{dp}(p_0)$$

are linear mappings from P to $I\!R^n$ resp. $I\!R^r$. By differentiating the boundary value problem (17)–(20) we obtain the following *linear* inhomogeneous BVP

$$\left.\begin{array}{rcll} \dot{y} &=& A^0(t)y + B^0(t)\eta + P^0(t) & , \\ \dot{\eta} &=& W^0(t)y - A^0(t)^*\eta + R^0(t) & , \\ y(a) &=& \varphi_p(p_0)\ ,\ \ \psi_x[b]y(b) + \psi_p[b] = 0 & , \\ \eta(b) &=& (g+\nu_0^*\psi)_{xx}[b]y(b) + \psi_x[b]^*\nu_p + (g+\nu_0^*\psi)_{xp}[b] & . \end{array}\right\} \qquad (35)$$

The matrices are defined on *interior arcs* $t \notin [t_1^0, t_2^0]$ by

$$\begin{aligned} &A^0(t), B^0(t), W^0(t) \quad \text{as in (29)} \quad , \\ &P^0(t) = f_p^0(t) - f_u^0(t) H_{uu}^0(t)^{-1} H_{up}^0(t) \quad , \\ &R^0(t) = H_{xu}^0(t) H_{uu}^0(t)^{-1} H_{up}^0(t) - H_{xp}^0(t) \ , \end{aligned} \tag{36}$$

and on the *boundary arc* $t \in [t_1^0, t_2^0]$ by

$$\begin{aligned} &A^0(t), B^0(t), W^0(t) \quad \text{as in (30)} \quad , \\ &P^0(t) = f_p^0(t) - f_u^0(t) C_u^0(t)^{-1} C_p^0(t) \quad , \\ &R^0(t) = \tilde{H}_{xu}^0(t) C_u^0(t)^{-1} C_p^0(t) - \tilde{H}_{xp}^0(t) \\ &\qquad + C_x^0(t) C_u^0(t)^{-1} (\tilde{H}_{up}^0(t) - \tilde{H}_{uu}^0(t) C_u^0(t)^{-1} C_p^0(t)) \ . \end{aligned} \tag{37}$$

The variation of the optimal control

$$v(t) := \frac{\partial u}{\partial p}\,(t, p_0) \tag{38}$$

is deduced from (26) using the derivatives in (10) and (11):

$$v(t) \;=\; -H_{uu}^0(t)^{-1}\{H_{ux}^0(t) y(t) + f_u^0(t)^* \eta(t) + H_{up}^0(t)\} \tag{39}$$

$$\text{for} \quad a \le t \le t_1^0 \quad \text{and} \quad t_2^0 \le t \le b \ ,$$

$$v(t) \;=\; -C_u^0(t)^{-1}\{C_x^0(t) y(t) + C_p^0(t)\} \ , \ t_1^0 \le t \le t_2^0 \ . \tag{40}$$

An explicit formula for the derivative dt_i/dp can be derived from the identity

$$\begin{aligned} &\tilde{C}(x(t_i(p),p), \lambda(t_i(p),p), p) = 0 \quad \text{for} \quad p \in V \ , \ i = 1,2 \ , \\ &\tilde{C}(x,\lambda,p) := C(x, u(x,\lambda,p), p) \ . \end{aligned}$$

Differentiation yields omitting arguments

$$(\tilde{C}_x \dot{x} + \tilde{C}_\lambda \dot{\lambda})\,\frac{dt_i}{dp} + \tilde{C}_x y + \tilde{C}_\lambda \eta + \tilde{C}_p = 0$$

which gives (compare Pesch 1989A, (65)):

$$\frac{dt_i}{dp}(p_0) = -(\tilde{C}_x y + \tilde{C}_\lambda \eta + \tilde{C}_p)(t_i^0) / \dot{C}(t_i^0) \ . \tag{41}$$

Here the denominator is nonzero due to **(A3)**. The next section will present two examples illustrating the use of the linear BVP (35) and the evaluation of (41).

6. Three numerical examples

The following three examples do not possess an analytical solution and will be solved numerically by the multiple shooting code BNDSCO developed in Bulirsch 1971, Oberle and Grimm 1989. All examples exhibit a *non-convex* Hamiltonian and hence sufficient conditions based on convexity do not apply. The check of optimality will then proceed via the existence of a solution of the Riccati ODE (31). For every example, the regularity of the shooting matrix $M[b]$ in (24) is verified by the code BNDSCO. We will strive for presenting a complete account of all assumptions and conditions developed in the preceding sections.

EXAMPLE 1 *The following control problem without inequality constraints admits two kinds of extremal solutions both with a nonsingular Jacobian for the shooting method. SSC single out only one solution as being optimal. For this solution a sensitivity analysis is performed as outlined in section 5. Consider the following classical variational problem depending on a parameter* $p \in I\!R$*:*

$$\textit{Minimize} \quad \frac{1}{2}\int_0^1 \{p \cdot x(t)^3 + \dot{x}(t)^2\}dt \tag{42}$$

$$\textit{subject to} \quad x(0) = 4\,, \quad x(1) = 1\,.$$

Defining as usual the control variable by $u := \dot{x}$ *the Hamiltonian becomes*

$$H(x, \lambda, u, p) = \frac{1}{2}(px^3 + u^2) + \lambda u\,.$$

The strict Legendre–Clebsch condition $H_{uu} = 1 > 0$ *in* **(A1)***(a) holds for all* p*. The function* u *in* **(A1)***(b) minimizing the Hamiltonian is the* C^∞*-function* $u(x, \lambda, p) = -\lambda$*. The parametric BVP (17) - (19) reduces to*

$$\ddot{x} = \frac{3}{2}px^2\,, \quad x(0) = 4\,, \quad x(1) = 1\,. \tag{43}$$

Unperturbed solution for $p_0 = 1$**.** *It can be shown by shooting methods (cf. Stoer and Bulirsch 1980, p. 170) that the BVP (43) with* $p = 1$ *has two solutions* $x_0(t) = 4/(1+t)^2$ *and* $x_1(t)$ *characterized by*

$$\dot{x}_0(0) = -8 \quad \textit{and} \quad \dot{x}_1(0) = -35.858549\,. \tag{44}$$

Both solutions are shown in Figure 1.

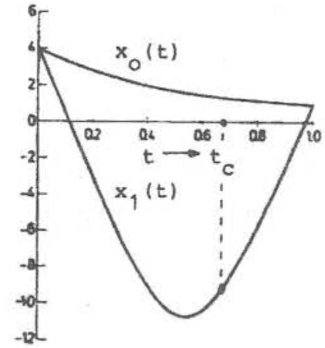

Figure 1. Solutions $x_0(t)$ and $x_1(t)$ for BVP (43); conjugate point $t_c = 0.674437$ for $x_1(t)$.

In order to test $x_0(t)$ and $x_1(t)$ for optimality with respect to (42) we can check the classical Jacobi-condition. The variational ODE for (43) along x_0 or x_1 becomes (compare also (28)):

$$\left.\begin{array}{llll} \ddot{x}_i = \frac{3}{2}x_i^2 & , \; x_i(0) = 4 & , \; \dot{x}_i(0) \;\; as\ in \;\; (44) & , \\ \ddot{y}_i = 3x_i(t)y_i & , \; y_i(0) = 0 & , \; \dot{y}_i(0) = 1 \quad (i = 0, 1) \, . & \end{array}\right\} \tag{45}$$

It can be verified by direct numerical integration that the classical Jacobi- condition holds along the solution x_0:

$$y_0(t) \neq 0 \quad for \quad 0 < t \leq 1 \, .$$

Hence x_0 is optimal for (42). Alternatively, optimality of x_0 can be verified by means of Theorem 4.1. The Riccati equation (32) becomes $\dot{Q} = -3x_0(t) + Q^2$. It is straightforward to compute a bounded solution Q in $[0, 1]$. On the other hand, for the solution x_1 we find that

$$y_1(t_c) = 0 \quad for \quad t_c = 0.674437 \, , \tag{46}$$

which means that the point $t_c \in (0, 1)$ is conjugate to $t = 0$. This violates the necessary condition of optimality in Zeidan and Zezza 1988, Theorem 3.1, and hence x_1 is non-optimal. We note that the exact value of the conjugate point t_c can be computed via the BVP (45) and (46) treating t_c as a free variable.

Perturbed solutions and sensitivity analysis. *By Theorem 5.1 there exists a neighborhood $V \subset I\!R$ of $p_0 = 1$ and a C^1-function $x(t, p)$ for $(t, p) \in [0, 1] \times V$ such that $x(\,\cdot\,, p)$ is optimal for (42) and satisfies $x(t, p_0) = x_0(t) = 4/(1 + t)^2$. It is easy to see that $x(t, p)$ is indeed a C^∞-function.*

Thus, we can consider the second-order Taylor expansion

$$x(t,p) = x_0(t) + \frac{\partial x}{\partial p}(t,p_0)(p-p_0) + \frac{1}{2}\frac{\partial^2 x}{\partial p^2}(t,p_0)(p-p_0)^2 + O(|p-p_0|^3)\ . \quad (47)$$

The sensitivity measures

$$z_1(t) := \frac{\partial x}{\partial p}(t,p_0) \quad resp. \quad z_2(t) = \frac{\partial^2 x}{\partial p^2}(t,p_0)$$

are solutions of the linear inhomogeneous BVPs

$$\begin{aligned} \ddot{z}_1 &\doteq 3x_0(t)z_1 + \tfrac{3}{2}x_0(t)^2\ , \quad z_1(0) = z_1(1) = 0\ , \\ \ddot{z}_2 &= 3x_0(t)z_2 + 3z_1(t)\{2x_0(t) + z_1(t)\}\ , \quad z_2(0) = z_2(1) = 0\ , \end{aligned}$$

which are obtained from (43) by differentiation with respect to p; compare also (35) and (36). The solution of these BVP's are given by

$$\dot{z}_1(0) = -3.779528 \quad resp. \quad \dot{z}_2(0) = 1.483277$$

from which the sensitivity approximation (47) can be generated.

EXAMPLE 2 *Consider the nonlinear control problem containing two parameters $p \in I\!R$ and $\alpha \in I\!R$: minimize*

$$\int_0^1 (u^2 - px^2)dt \quad (48)$$

subject to

$$\dot{x} = x^2 - u\ ,\ x(0) = 1\ ,\ x(1) = 1 \quad (49)$$

$$x + u \le \alpha\ . \quad (50)$$

The nominal parameter values are $p_0 = 10$ and $\alpha_0 = 5.9$. The choice of α_0 will become clear after studying the unconstrained problem (48), (49) .

Unconstrained solution depending on $p \in I\!R$.

The Hamiltonian $H = u^2 - px^2 + \lambda(x^2 - u)$ satisfies assumption **(A1)** *with $H_{uu} = 2$ and minimizing control $u(x,\lambda,p) = \lambda/2$ which is obtained from $H_u = 0$. The parametric $BVP(p)$ is*

$$\dot{x} = x^2 - 0.5\lambda\ , \quad \dot{\lambda} = 2x(p-\lambda)\ ,\ x(0) = 1\ ,\ \ x(1) = 1\ . \quad (51)$$

The shooting method yields the unperturbed solution

$$\lambda_0(0) = -5.347274985 \qquad for \quad p_0 = 10\ .$$

The unconstrained solution is denoted by $x_0(t)$, $u_0(t)$. *The function* $C^0(t) = x_0(t) + u_0(t)$ *attains its maximum at*

$$\begin{aligned} \overline{\alpha} &:= \max_{0 \le t \le 1} \{x_0(t) + u_0(t)\} = x_0(t_1) + u_0(t_1) = 6.017207420 \, , \\ t_1 &= 0.7830404341 \, . \end{aligned}$$

Hence for $\alpha = \alpha_0 = 5.9 < \overline{\alpha}$ *the constraint (50) becomes active.*
The Riccati equation (32) is

$$\dot{Q} = -4x_0(t)Q + 20 - 2\lambda_0(t) + 0.5Q^2 \, .$$

With $Q(0) = 0$ *this equation has a finite solution* $Q(t) \in [0., 4.]$ *for* $0 \le t \le 1$. *Hence* x_0, u_0 *are optimal by Theorem 4.1. By Theorem 5.1 we can embed* x_0, u_0, λ_0 *into an optimal* C^1*-family* $x(t,p), u(t,p), \lambda(t,p)$ *for* p *near* $p_0 = 10$. *The system (35) for* $y(t) = \partial x(t,p_0)/\partial p$, $\eta(t) := \partial\lambda(t,p_0)/\partial p$ *is obtained by differentiating (51):*

$$\left. \begin{aligned} \dot{y} &= 2x_0 y - 0.5\eta \quad , \\ \dot{\eta} &= 2\{y(p_0 - \lambda_0) + x_0(1-\eta)\} \quad , \\ y(0) &= 0 \, , \; y(1) = 0 \quad . \end{aligned} \right\} \tag{52}$$

Computation yields the initial value

$$\eta(0) = -1.016091005 \, .$$

The control variation (38) then becomes $v(t) = 0.5\eta(t)$.

Constrained solution with $\alpha_0 = 5.9$ and parameter p.

We can expect that the constraint $x + u \le \alpha_0 = 5.9$ *will lead to one boundary arc with* $0 < t_1^0 < t_2^0 < 1$. *The augmented Hamiltonian is*

$$\tilde{H} = u^2 - px^2 + \lambda(x^2 - u) + \mu(x + u - \alpha_0) \, .$$

Assumption **(A2)** *holds with* $C(x,u,p) = x + u - \alpha_0$, $C_u = 1$ *and* $u_b(x,p) = \alpha_0 - x$. *The multiplier* μ *in (13) becomes*

$$\mu(x,\lambda,p) = -H_u/C_u = -2u_b(x,p) + \lambda = 2(x - \alpha_0) + \lambda \, .$$

The parametric $BVP(p)$ *in (17) - (20) can be stated explicitly:*

$$\dot{x} = \begin{cases} x^2 - 0.5\lambda & , \quad t \notin [t_1, t_2] \\ x^2 + x - \alpha_0 & , \quad t \in [t_1, t_2] \end{cases} \tag{53}$$

$$\dot{\lambda} = \begin{cases} 2x(p - \lambda) & , \quad t \notin [t_1, t_2] \\ 2x(p - \lambda) - \mu & , \quad t \in [t_1, t_2] \\ \mu = 2(x - \alpha_0) + \lambda & \end{cases} \tag{54}$$

$$x(0) = 1 \, , \;\; x(1) = 1 \, , \;\; x(t_i) + 0.5\lambda(t_i) = \alpha_0 \, , \quad i = 1, 2 \, .$$

The solution for $\alpha_0 = 5.9$ *and* $p_0 = 10$ *is*

$$\lambda_0(0) = -5.324898490\ ,\ \ t_1^0 = 0.6735245190\ ,\ \ t_2^0 = 0.8988553586\ .$$

It is easy to verify that the Riccati ODE (31)

$$\dot{Q} = \begin{cases} -4x_0(t)Q + 20 - 2\lambda_0(t)) + 0.5Q^2 & ,\quad t \notin [t_1^0, t_2^0] \\ (-4x_0(t) - 2)Q + 18 - 2\lambda_0(t) & ,\quad t \in [t_1^0, t_2^0] \end{cases}$$

has a finite solution Q *on* $[0,1]$. *Thus the unperturbed solution* $x_0(t)$, $\lambda_0(t)$, $u_0(t) = \lambda_0(t)/2$ *is optimal. Moreover, assumption* **(A3)** *on the non-tangential junction holds with* $C^0(t) = x_0(t) + u_0(t)$ *and*

$$\dot{C}^0(t_1^0) = 1.848039743\ ,\ \ \dot{C}^0(t_2^0) = -1.673196320\ .$$

The multiplier $\mu_0(t)$ *satisfies*

$$\dot{\mu}_0(t_1^0) = 3.696079485\ ,\ \ \dot{\mu}_0(t_2^0) = -3.346392641\ ,$$
$$\mu_0(t) > 0 \qquad \text{for} \quad t_1^0 < t < t_2^0\ .$$

Hereby all assumption for solution differentiability in Theorem 5.1 have been checked. The linear inhomogeneous BVP for $y(t) = \partial x(t, p_0)/\partial p$ *and* $\eta(t) = \partial\lambda(t, p_0)/\partial p$ *can be deduced from differentiation of (53) and (54). The ODE agrees with (52) on interior arcs and is given on the boundary arc* $t_1^0 \le t \le t_2^0$ *by*

$$\dot{y} = 2x_0 y + y, \quad \dot{\eta} = 2\{y(p_0 - \lambda_0) + x_0(1 - \eta)\} - \eta - 2y\ .$$

The solution is complete by computing

$$\eta(0) = -0.8595770938\ .$$

The optimal control variation then is found from $v(t) = \eta(t)/2$ *on interior arcs and from* $v(t) = -y(t)$ *on the boundary arc. Finally, since* $C(x, \lambda, p) = x + 0.5\lambda$ *formula (41) yields* $dt_i(p_0)/dp = -(y + 0.5\eta)/(\dot{x} + 0.5\dot{\lambda})|_{t_i^0}$ *which gives*

$$\frac{dt_1}{dp}(p_0) = -0.2557112952\ , \qquad \frac{dt_2}{dp}(p_0) = 0.2671182925\ .$$

Constrained solution with $p_0 = 10$ and parameter α.

The unperturbed solution $x_0(t), \lambda_0(t)$ *with* $p_0 = 10$ *and* $\alpha_0 = 5.9$ *can be embedded into a* C^1*-familiy* $x(t,\alpha), \lambda(t,\alpha)$ *of optimal solutions to problem (48) - (50) with* $p = p_0 = 10$ *and* α *near* α_0. *On the boundary* $t_1^0 \le t \le t_2^0$ *the ODEs now are*

$$\dot{x} = x^2 + x - \alpha\ ,\quad \dot{\lambda} = 2x(p_0 - \lambda) - \mu\ ,\ \ \mu(x, \lambda, \alpha) = 2(x - \alpha) + \lambda\ .$$

Hence, the linear inhomogeneous BVP for the variations $y(t) = \partial x(t, \alpha_0)/\partial \alpha$, $\eta(t) = \partial \lambda(t, \alpha_0)/\partial \alpha$ *turns out to be*

$$\dot{y} = \begin{cases} 2x_0 y - 0.5\eta & , \quad t \notin [t_1^0, t_2^0] \\ 2x_0 y + y - 1 & , \quad t \in [t_1, t_2^0] \end{cases}$$

$$\dot{\eta} = \begin{cases} 2\{y(p_0 - \lambda_0) - x_0\eta\} & , \quad t \notin [t_1^0, t_2^0] \\ 2\{y(p_0 - \lambda_0) - x_0\eta\} - \eta - 2y + 2 & , \quad t \in [t_1, t_2^0] \end{cases}$$

$$y(0) = 0 \, , \quad y(1) = 0 \, .$$

The computed initial value is

$$\eta(0) = -0.2717521464 \, .$$

The variations of junctions points are found from (41) where now $\tilde{C}(x, \lambda, \alpha) = x + 0.5\lambda - \alpha$*:*

$$\begin{aligned} \frac{dt_i}{d\alpha}(\alpha_0) &= (1 - y - 0.5\eta)/(\dot{x} + 0.5\dot{\lambda})|_{t_i^0} \, , \quad i = 1, 2 \, , \\ \frac{dt_1}{d\alpha}(\alpha_0) &= 0.4330244699 \, , \quad \frac{dt_2}{d\alpha}(\alpha_0) = -0.4869079015 \, . \end{aligned}$$

EXAMPLE 3 (A plug–flow tubular reactor with a perturbed control constraint) *Fan 1966, Chapter 4, describes models for a plug–flow tubular reactor in which the reaction* $A \to B \to C$ *takes place where* B *is the desired product. Let* $x_1(t)$ *and* $x_2(t)$ *designate the concentrations of* A *and* B*, respectively, along the length* t *of the reactor,* $0 \le t \le 1$*. The problem is to determine the temperature profile* $T(t)$ *which maximizes the concentration* $x_2(1)$ *at the reactor outlet. We introduce a new control variable* $u(t) := exp\,(-\alpha/T(t))$, $\alpha > 0$*, and consider the problem of minimizing the cost function*

$$J(x, u, p) = -x_2(1) \tag{55}$$

subject to

$$\begin{aligned} \dot{x}_1 &= -ux_1 + u^2 x_2 \quad , \quad x_1(0) = 1 \quad , \\ \dot{x}_2 &= ux_1 - 3u^2 x_2 \quad , \quad x_2(0) = 0 \quad , \end{aligned} \tag{56}$$

$$u(t) \le p \, , \quad 0 \le t \le 1 \tag{57}$$

The reference parameter is $p_0 = 1$*. The Hamiltonian*

$$H = \lambda_1(-ux_1 + u^2 x_2) + \lambda_2(ux_1 - 3u^2 x_2)$$

is not convex in the variables x_1, x_2, u. *The control which minimizes* H *is computed from* $H_u = 0$ *as*

$$u(x,\lambda) = \frac{(\lambda_1 - \lambda_2)x_1}{2(\lambda_1 - 3\lambda_2)x_2} \,. \tag{58}$$

Since $x_2(0) = 0$, *the control constraint (57) will become active for* $0 \le t \le t_1$. *We shall compute the optimal control assuming the structure*

$$u(t) = \begin{cases} p & , \quad 0 \le t \le t_1 \\ u(x(t),\lambda(t)) & , \quad t_1 \le t \le 1 \,. \end{cases} \tag{59}$$

The adjoint equations (18) and the transversality conditions (16) are

$$\begin{aligned} \dot\lambda_1 &= (\lambda_1 - \lambda_2)u \quad , & \lambda_1(1) &= 0 \;, \\ \dot\lambda_2 &= (3\lambda_2 - \lambda_1)u^2 \quad , & \lambda_2(1) &= -1 \;. \end{aligned} \tag{60}$$

The junction condition simply is

$$u(x(t_1),\lambda(t_1)) = p \,. \tag{61}$$

For $p_0 = 1$ *the unperturbed solution* $x^0(\,\cdot\,), \lambda^0(\,\cdot\,), u_0(\,\cdot\,)$ *of (56) - (61) is given by (compare Figure 2)*

$$\begin{aligned} \lambda_1^0(0) &= -0.2881047867 \quad , \quad \lambda_2^0(0) = -0.3962607822 \,, \\ t_1^0 &= 0.1058506650 \quad . \end{aligned}$$

The junction at t_1^0 *is non–tangential since*

$$\dot u_0((t_1^0)^+) = -5.353944361 \,. \tag{62}$$

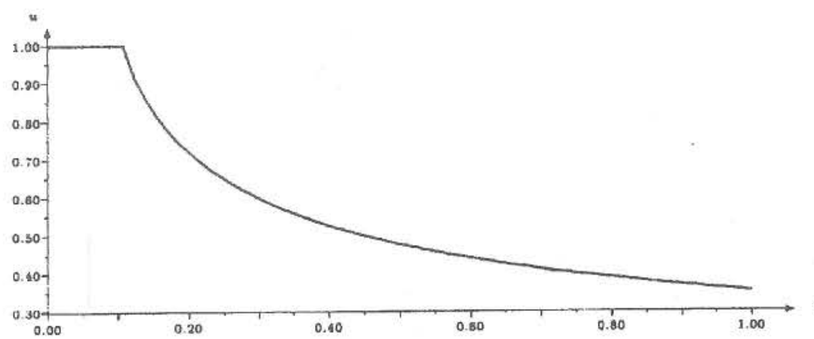

Figure 2. Unperturbed optimal control $u_0(t)$ with non–tangential junction at $t_1^0 = 0.10585$.

The strict Legendre–Clebsch condition **(A1)(a)** *holds with*

$$H^0_{uu}(t) = 2(\lambda^0_1(t) - 3\lambda^0_2(t))x^0_2(t) \geq 0.1 \quad for \quad t^0_1 \leq t \leq 1 .$$

It is interesting to note that the strict Legendre–Clebsch condition is violated at $t = 0$ *since* $x_2(0) = 0$ *and* $H^0_{uu}(0) = 0$. *Hence strong SSC which would require the existence of a solution of the Riccati ODE (32) on the whole interval* $[0, 1]$ *are not satisfied. However, one can check that the Riccati ODE (31) has a bounded* 2×2*-matrix solution on* $[0, 1]$ *since (31) reduces to the linear ODE (33) on* $[0, t^0_1]$. *In fact, the symmetric solution* $Q(t)$ *with*

$$Q(t) = \begin{pmatrix} q_1(t) & q_2(t) \\ q_2(t) & q_4(t) \end{pmatrix} , \qquad Q(1) = 0 \quad ,$$

satisfies the boundary condition (34) and is bounded by $|q_i(t)| \leq 7$ *for* $0 \leq t \leq 1$. *We then conclude that the triple* x^0, λ^0, u_0 *is optimal and meets all assumptions for solution differentiability in Theorem 5.1.*

The linear BVP for the variations $y(t) = \partial x(t, p_0)/\partial p \in \mathbb{R}^2$ *and* $\eta(t) = \partial \lambda(t, p_0)/\partial p \in \mathbb{R}^2$ *with respect to the perturbation p in (57) will be stated explicitly now. On the boundary* $[0, t^0_1]$ *we set* $u = p$ *and differentiate (56) and (60):*

$$\begin{aligned} \dot y_1 &= -y_1 - x^0_1 + y_2 + 2x^0_2 \quad , & y_1(0) &= 0 \ , \\ \dot y_2 &= y_1 + x^0_1 - 3y_2 - 6x^0_2 \quad , & y_2(0) &= 0 \ , \\ \dot \eta_1 &= \eta_1 - \eta_2 + \lambda^0_1 - \lambda^0_2 \quad , & \eta_1(1) &= 0 \ , \\ \dot \eta_2 &= 3\eta_2 - \eta_1 + 2(3\lambda^0_2 - \lambda^0_1) \quad , & \eta_2(1) &= 0 \ . \end{aligned}$$

On the interior arc $[t^0_1, 1]$ *we have to differentiate (56) and (60) using the control expression (58): let*

$$\begin{aligned} K^0 &:= H^0_{uu} = 2(\lambda^0_1 - 3\lambda^0_2)x^0_2 \quad , \\ u_{x_1} &= (\lambda^0_1 - \lambda^0_2)/K^0 \ , \ u_{x_2} = (\lambda^0_2 - \lambda^0_1)x^0_1/(K^0 x^0_2) \quad , \\ u_{\lambda_1} &= \{x^0_1 + 2(\lambda^0_2 - \lambda^0_1)x^0_1 x^0_2/K^0\}/K^0 \quad , \\ u_{\lambda_2} &= \{-x^0_1 + 6(\lambda^0_1 - \lambda^0_2)x^0_1 x^0_2/K^0\}/K^0 \quad , \\ \frac{du}{dp} &= DUP := u_{x_1}y_1 + u_{x_2}y_2 + u_{\lambda_1}\eta_1 + u_{\lambda_2}\eta_2 \quad , \end{aligned}$$

then

$$\begin{aligned} \dot y_1 &= -u_0 y_1 + u_0^2 y_2 + DUP(-x^0_1 + 2u_0 x^0_2) \quad , \\ \dot y_2 &= u_0 y_1 - 3u_0^2 y_2 + DUP(x^0_1 - 6u_0 x^0_2) \quad , \\ \dot \eta_1 &= (\eta_1 - \eta_2)u_0 + (\lambda^0_1 - \lambda^0_2)DUP \quad , \\ \dot \eta_2 &= (3\eta_2 - \eta_1)u_0^2 + (6\lambda^0_2 - 2\lambda^0_1)u_0 DUP \quad . \end{aligned}$$

The computed initial values for η *are*

$$\eta_1(0) = -0.005964209117 \ , \ \eta_2(0) = 0.1112586737 \ .$$

The variation of the junction point $t_1(p)$ can be obtained explicitly observing (41), (61) and the definition of DUP above:

$$\frac{dt_1}{dp}(p_0) = \frac{1 - DUP}{\dot{u}_0((t_1^0)^+)} = -0.2802828805 \ .$$

To allow for a comparison with numerical differentiation we take $p = p_0 + 10^{-4}$ and compute

$$t_1(1.0001) = 0.1058226418 \ .$$

The difference quotient

$$(t_1(1.0001) - t_1(1)) \cdot 10^4 = -0.280243$$

approximates the exact derivative by four digits.

7. Conclusion

Parametric nonlinear control problems with control–state constraints have been considered in this paper. Full solution differentiability of the optimal solution and of the adjoint variable has been obtained under assumptions which are inspired by numerical experience. These assumptions are slightly stronger than the ones used by other authors who restrict the discussion to pure control constraints.

A further distinction to other approaches in sensitivity and stability is that our approach is closely related to numerical shooting methods for solving the associated boundary value problem (BVP). Shooting methods generate a family of extremal solutions which can be considered as an extension of field theory in the classical calculus of variations. The nonsingularity of the Jacobian for the shooting procedure is related to properties of the variational system corresponding to the BVP. We have mapped a direct route leading from the variational system to recently developed second–order sufficient conditions (SSC) via a Riccati ODE. The additional assumption **(A3)** on non-tangential junctions with the boundary is a new element brought about by the inequality constraint.

We have assumed that the control and the inequality constraint are *scalar*. In many practical applications it suffices to consider the following vector–valued situation to which our results immediately carry over: let $u \in I\!R^m$ and $C : I\!R^{n+m} \times P \rightarrow I\!R^s$. Then each component C_i depends only on one control component u_k such that $\partial C_i / \partial u_k \neq 0 \ , \quad \partial C_i / \partial u_j = 0 \quad \text{for} \quad j \neq k$.

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