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INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

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A well-posed shooting algorithm for optimal control problems with singular arcs

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Abstract: In this article we establish for the first time the well-posedness of the shooting algorithm applied to optimal control problems for which all control variables enter linearly in the Hamiltonian. We start investigating the case having only initial-final state constraints and free control variable, and afterwards we deal with control bounds. The shooting algorithm is well-posed if the derivative of its associated shooting function is injective at the optimal solution. The main result of this paper is to provide a sufficient condition for this injectivity, that is very close to the second order necessary condition. We prove that this sufficient condition guarantees the stability of the optimal solution under small perturbations and the well-posedness of the shooting algorithm for the perturbed problem. We present numerical tests that validate our method.

Key-words: optimal control, Pontryagin Maximum Principle, singular control, constrained control, shooting algorithm, second order optimality condition, stability

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Un algorithme de tir bien posé pour les problèmes de commande optimale avec des arcs singuliers

Résumé : Dans ce travail on présente pour la première fois une condition suffisante pour que l'algorithme de tir soit bien posé quand il est appliqué aux problèmes de commande optimale affines dans les commandes. On commence par étudier le cas avec des contraintes initiales-finales sur l'état et commande libre, et ensuite on ajoute des contraintes sur la commande. L'algorithme de tir est bien posé si la dérivée de la fonction de tir associée est injective dans la solution optimale. Le résultat principal de cet article montre une condition suffisante pour cette injectivité, qui est très proche de la condition nécessaire du second ordre. On montre que cette condition suffisante assure la stabilité de la solution optimale aux petites perturbations et qu'elle garantit aussi que l'algorithme de tir est bien posé pour le problème perturbé. On présente des essais numériques qui valident notre méthode.

Mots-clés : commande optimale, Principe de Pontryaguine, commande singulière, contraintes sur la commande, algorithme de tir, conditions d'optimalité du second ordre, stabilité

1 Introduction

In this article we study the well-posedness of the shooting algorithm applied to optimal control problems for which all control variables enter linearly in the Hamiltonian. We start investigating the case having only initial-final state constraints and free control variable, and afterwards we deal with control bounds.

Some references can be mentioned regarding the shooting method. The first two works we can find in the literature, dating from years 1956 and 1962 respectively, are Goodman-Lance [21] and Morrison et al. [32]. Both present the same method for solving two-point boundary value problems in a general setting, not necessarily related to an optimal control problem. The latter article applies to more general formulations. The method was studied in detail in Keller's book [22], and later on Bulirsch [7] applied it to the resolution of optimal control problems.

The case we deal with in this paper, where the shooting method is used to solve optimal control problems having bang-singular solutions, is treated in Maurer [30], Fraser-Andrews [16] and Martinon PhD thesis [27]. They all provide a series of algorithms and numerical examples with different control structures, but no theoretical foundation is supplied.

Concerning the well-posedness of the shooting method in optimal control problems, Malanowski-Maurer [26] and Bonnans-Hermant [6] deal with a problem having mixed control-state and pure state running constraints and satisfying the strong Legendre-Clebsch condition.

We start the article by presenting an optimal control problem affine in the control, with terminal constraints and free control variables. For this kind of problem we state a set of optimality conditions which is equivalent to the Pontryagin Maximum Principle. Afterwards, the second order strengthened generalized Legendre-Clebsch condition is used to eliminate the control variable from the stationarity condition. The resulting set of conditions turns out to be a two-point boundary value problem, i.e., a system of ordinary differential equations having boundary conditions both in the initial and final times. We define the shooting function as the mapping that assigns to each estimate of the initial values, the value of the final condition of the corresponding solution. The shooting algorithm consists of approximating a zero of this function. In other words, the method finds suitable initial values for which the corresponding solution of the differential equation system satisfies the final conditions.

Since the number of equations happens to be, in general, greater than the number of unknowns, the Gauss-Newton method is a suitable approach for solving this overdetermined system of equations. The reader is referred to Dennis [9], Fletcher [15] and Dennis et al. [10] for details and implementations of Gauss-Newton technique. This method is applicable when the derivative of the shooting function is one-to-one at the solution, and in this case it converges quadratically.

The main result of this paper is to provide a sufficient condition for the injectivity of this derivative, and to notice that this condition is quite weak since, for qualified problems, it characterizes quadratic growth in the weak sense (see Dmitruk [11, 12]). Once the unconstrained case is investigated, we pass to a problem having bounded controls. To treat this case, we perform a transformation yielding a new problem without bounds, we prove that an optimal solution

of the original problem is also optimal for the transformed one and we apply our well-posedness result to this modified formulation.

It is interesting to mention that by means of the latter result we can justify, in particular, the well-posedness of the algorithm proposed by Maurer [30]. In this work, Maurer suggested a method to treat problems having scalar bang-singular-bang solutions and provided a square system of (nonlinear) equations meant to be solved by Newton's algorithm. However, the systems that can be encountered in practice are not always square and hence need to be tackled with our approach.

We investigate the stability of the optimal solution in both unconstrained and constrained control cases. It is shown that the sufficient condition mentioned above guarantees the stability of the optimal solution under small perturbation of the data, as well as the well-posedness of the shooting algorithm for the perturbed problem. Felgenhauer in [14, 13] provided sufficient conditions for the stability of the structure of the optimal control, but assuming that the perturbed problem had an optimal solution.

Our article is organized as follows. In the first section we present the optimal control problem without bound constraints, for which we provide an optimality system in the second section. We give a description of the shooting method in the third section. In the fourth section we present a set of second order necessary and sufficient conditions, and the statement of the main result. We introduce a linear quadratic optimal control problem in section 6. In section 7 we present a variable transformation relating the shooting system and the optimality system of the linear quadratic problem mentioned above. In section 8 we deal with the control constrained case. A stability analysis for both unconstrained and constrained control cases is provided in section 9. Finally we present some numerical tests in section 10, and we devote section 11 to the conclusions of the article.

2 Statement of the problem

Consider the spaces $\mathcal{U} := L_\infty(0, T; \mathbb{R}^m)$ and $\mathcal{X} := W_\infty^1(0, T; \mathbb{R}^n)$, as control and state spaces, respectively. Denote by u and x their elements, respectively. When needed, put $w = (x, u)$ for a point in the product space $\mathcal{W} := \mathcal{X} \times \mathcal{U}$. In this paper we investigate the optimal control problem

$$J := \varphi_0(x_0, x_T) \rightarrow \min, \quad (1)$$

$$\dot{x}_t = \sum_{i=0}^m u_{i,t} f_i(x_t), \quad \text{for } t \in (0, T), \quad (2)$$

$$\eta_j(x_0, x_T) = 0, \quad \text{for } j = 1, \dots, d_\eta, \quad (3)$$

where final time T is fixed, $u_0 \equiv 1$, $f_i : \mathbb{R}^n \rightarrow \mathbb{R}^n$ for $i = 0, \dots, m$ and $\eta_j : \mathbb{R}^{2n} \rightarrow \mathbb{R}$ for $j = 1, \dots, d_\eta$. Assume that data functions φ_0 , f_i and η_j are twice continuously differentiable. Denote by (P) the problem defined by equations (1) to (3). An element $w \in \mathcal{W}$ satisfying (2)-(3) is called *feasible trajectory*.

Set $\mathcal{X}_* := W_\infty^1(0, T; \mathbb{R}^{n,*})$ the space of Lipschitz continuous functions with values in the n -dimensional space of row-vectors with real components $\mathbb{R}^{n,*}$. Consider an element $\lambda := (\alpha_0, \beta, p) \in \mathbb{R} \times \mathbb{R}^{d_\eta,*} \times \mathcal{X}_*$ and define the *pre-*

Hamiltonian function

$$H[\lambda](x, u, t) := p_t \sum_{i=0}^m u_i f_i(x), \quad (4)$$

the *initial-final Lagrangian function*

$$\ell[\lambda](\zeta_0, \zeta_T) := \alpha_0 \varphi_0(\zeta_0, \zeta_T) + \sum_{j=1}^{d_\eta} \beta_j \eta_j(\zeta_0, \zeta_T), \quad (5)$$

and the *Lagrangian function*

$$\mathcal{L}[\lambda](w) := \ell[\lambda](x_0, x_T) + \int_0^T p_t \left(\sum_{i=0}^m u_{i,t} f_i(x_t) - \dot{x}_t \right) dt. \quad (6)$$

We study a nominal feasible trajectory $\hat{w} = (\hat{x}, \hat{u})$.

Definition 2.1. An element $\lambda = (\alpha_0, \beta, p) \in \mathbb{R}_+ \times \mathbb{R}^{d_\eta, *}$ is a *Pontryagin multiplier* if it satisfies the *Pontryagin Maximum Principle*, i.e., if p is solution of the *costate equation*

$$-\dot{p}_t = D_x H[\lambda](\hat{x}_t, \hat{u}_t, t), \quad \text{on } [0, T], \quad (7)$$

with the *transversality conditions*

$$p_0 = -D_{x_0} \ell[\lambda](\hat{x}_0, \hat{x}_T), \quad (8)$$

$$p_T = D_{x_T} \ell[\lambda](\hat{x}_0, \hat{x}_T), \quad (9)$$

and the following *minimum condition* holds:

$$H[\lambda](\hat{x}(t), \hat{u}(t), t) = \min_{v \in \mathbb{R}^m} H[\lambda](\hat{x}(t), v, t), \quad \text{a.e. on } [0, T]. \quad (10)$$

Assumption 2.2. \hat{w} has a unique associated multiplier denoted by $\hat{\lambda} = (\hat{p}, \hat{\alpha}_0, \hat{\beta})$.

This implies that \hat{w} verifies the classical *qualification hypothesis*: the function that associates to each $(z_0, v) \in \mathbb{R}^n \times \mathcal{U}$ the value $D\eta(\hat{x}_0, \hat{x}_T)(z_0, z_T) \in \mathbb{R}^{d_\eta}$ is surjective. In other words, $D\eta(\hat{x}_0, \hat{x}_T)$ is onto when considered as a function of (z_0, v) . And hence, \hat{w} is a *normal extremal*, i.e., $\hat{\alpha}_0 > 0$. In particular, we may assume

$$\hat{\alpha}_0 = 1. \quad (11)$$

Let the *switching function* $\Phi : [0, T] \rightarrow \mathbb{R}^{m, *}$ be defined by

$$\Phi_t := D_u H[\hat{\lambda}](\hat{x}_t, \hat{u}_t, t) = (\hat{p}_t f_i(\hat{x}_t))_{i=1}^m. \quad (12)$$

Observe that the minimum condition (10) is equivalent to

$$\Phi_t = 0, \quad \text{a.e. on } [0, T]. \quad (13)$$

3 Optimality system

This section provides an optimality system for \hat{w} in terms of the Pontryagin Maximum Principle presented above.

In the sequel assume that the trajectory \hat{w} is a *weak minimum* of problem (P), i.e., there exists $\varepsilon > 0$ such that \hat{w} is a minimum in the set of feasible trajectories $w = (x, u) \in \mathcal{W}$ satisfying

$$\|x - \hat{x}\|_\infty < \varepsilon, \quad \|u - \hat{u}\|_\infty < \varepsilon.$$

Observe that, since H is affine in the control, the switching function Φ introduced in (12) does not depend explicitly on u . Let an index $i = 1, \dots, m$, and $(d^{M_i}\Phi/dt^{M_i})$ be the lowest order derivative of Φ in which u_i appears with a coefficient that is not identically zero on $(0, T)$. In Kelley et al. [24] it is stated that M_i is even, assuming that the extremal is normal, i.e., 11 holds. The integer $N_i := M_i/2$ is called *order of the singular arc*.

Assumption 3.1. *The strengthened generalized Legendre condition (see Kelley [23] and Goh [19]) holds, i.e.,*

$$-\frac{\partial}{\partial u} \ddot{\Phi} \succ 0. \quad (14)$$

Hence, the order of \hat{u}_i is 1 for every $i = 1, \dots, m$, and we can solve \hat{u} in terms of \hat{x} and \hat{p} , from equation

$$\ddot{\Phi} = 0, \quad \text{a.e. on } (0, T). \quad (15)$$

Let us compute $\dot{\Phi}$ and $\ddot{\Phi}$. Denote the Lie bracket of two smooth vector fields $g, h : \mathbb{R}^n \rightarrow \mathbb{R}^n$ by

$$[g, h](x) := g'(x)h(x) - h'(x)g(x). \quad (16)$$

Define $A : \mathbb{R}^{n+m} \rightarrow \mathcal{M}_{n \times n}(\mathbb{R})$ and $B : \mathbb{R}^n \rightarrow \mathcal{M}_{n \times m}(\mathbb{R})$ by

$$A(x, u) := \sum_{i=0}^m u_i f'_i(x), \quad B(x)v := \sum_{i=1}^m v_i f_i(x), \quad (17)$$

for every $v \in \mathbb{R}^m$. For $(x, u) \in \mathcal{W}$ satisfying (2), let

$$B_1(x_t, u_t) := A(x_t, u_t)B(x_t) - \frac{d}{dt}B(x_t). \quad (18)$$

Easily follows that B_1 does not depend on u_t and thus, $B_1 : \mathbb{R}^n \rightarrow \mathcal{M}_{n \times m}(\mathbb{R})$. Note that

$$\dot{\Phi}_t = p_t B(x_t), \quad \dot{\Phi}_t = -p_t B_1(x_t). \quad (19)$$

An optimality system for problem (P) is composed by equations (2)-(3), (7)-(9) together with condition (13). Note that the latter is equivalent to (15) and the endpoint conditions

$$\Phi_T = 0, \quad \dot{\Phi}_0 = 0. \quad (20)$$

Use (19) to rewrite (20) as follows:

$$p_T B(x_T) = 0, \quad (21)$$

$$p_0 B_1(x_0) = 0. \quad (22)$$

Notation: Denote by (OS) the set of equations composed by (2)-(3), (7)-(9), (15), (21)-(22).

Note that, since (15) holds, conditions (21)-(22) are imposed in order to guarantee (13). We could choose another pair of endpoint conditions among the four possible ones: $\Phi_0 = 0$, $\Phi_T = 0$, $\dot{\Phi}_0 = 0$ and $\dot{\Phi}_T = 0$, always including at least one of order zero. The choice we made will simplify the presentation of the result afterwards.

4 Shooting Algorithm

The aim of this section is to present an appropriated numerical scheme to solve system (OS). For this purpose define the *shooting function*:

$$\mathcal{S} : \mathcal{D}(\mathcal{S}) := \mathbb{R}^n \times \mathbb{R}^{n+d_\eta,*} \rightarrow \mathbb{R}^{d_\eta} \times \mathbb{R}^{2n+2m,*},$$

$$(x_0, p_0, \beta) =: \nu \mapsto \mathcal{S}(\nu) := \begin{pmatrix} \eta(x_0, x_T) \\ p_0 + D_{x_0} \ell[\lambda](x_0, x_T) \\ p_T - D_{x_T} \ell[\lambda](x_0, x_T) \\ p_T B(x_T) \\ p_0 B_1(x_0) \end{pmatrix}, \quad (23)$$

where (x, u, p) is a solution of (2), (7), (15) with initial conditions x_0 and p_0 , and $\lambda := (\beta, p)$. We denote either by (a_1, a_2) or $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ an element of the product space $A_1 \times A_2$. Observe that in a simpler framework having fixed initial state and no final constraints, the shooting function depends only on p_0 . In our case, since the initial state is not fixed and a multiplier associated to the initial-final constraints must be considered, \mathcal{S} has more independent variables. Note that solving (OS) consists of finding $\nu \in \mathcal{D}(\mathcal{S})$ such that

$$\mathcal{S}(\nu) = 0. \quad (24)$$

This procedure is called the *shooting method*. Since the number of equations in (24) is greater than the number of unknowns, the Gauss-Newton method is a suitable approach to solve it. This algorithm will solve the equivalent least squares problem

$$\min_{\nu \in \mathcal{D}(\mathcal{S})} |\mathcal{S}(\nu)|^2. \quad (25)$$

At each iteration k , given the approximate values ν^k we look for Δ^k that gives the minimum of the linear approximation of problem

$$\min_{\Delta \in \mathcal{D}(\mathcal{S})} |\mathcal{S}(\nu^k) + \mathcal{S}'(\nu^k)\Delta|^2. \quad (26)$$

Afterwards we update

$$\nu^{k+1} \leftarrow \nu^k + \Delta^k. \quad (27)$$

In order to solve the problem in (26) at each iteration k , we look for Δ in the kernel of the derivative of the objective function, i.e., Δ satisfying

$$\mathcal{S}'(\nu^k)^\top \mathcal{S}'(\nu^k)\Delta + \mathcal{S}'(\nu^k)^\top \mathcal{S}(\nu^k) = 0. \quad (28)$$

Hence, in order to compute direction Δ matrix $\mathcal{S}'(\nu^k)^\top \mathcal{S}'(\nu^k)$ must be nonsingular. Thus, Gauss-Newton method will be applicable or *well-posed* provided that $\mathcal{S}'(\hat{\nu})^\top \mathcal{S}'(\hat{\nu})$ is invertible, where $\hat{\nu} := (\hat{x}_0, \hat{p}_0, \hat{\beta})$. Easily follows that $\mathcal{S}'(\hat{\nu})^\top \mathcal{S}'(\hat{\nu})$ is nonsingular if and only if $\mathcal{S}'(\hat{\nu})$ is one-to-one.

The main result of this article is presenting a condition that guarantees the well-posedness of the shooting method around the optimal local solution $(\hat{w}, \hat{\lambda})$. This condition involves the second variation studied in Dmitruk [11, 12], more precisely, the sufficient optimality conditions therein presented.

4.1 Linearization of a Differential Algebraic System

For the aim of finding an expression of $\mathcal{S}'(\hat{\nu})$, we make use of the linearization of (OS) and thus we introduce the following concept:

Definition 4.1 (Linearization of a Differential Algebraic System). *Consider a system of differential algebraic equations:*

$$\dot{\zeta}_t = \mathcal{F}(\zeta_t, \alpha_t), \quad (29)$$

$$0 = \mathcal{G}(\zeta_t, \alpha_t), \quad (30)$$

$$0 = \mathcal{I}(\zeta_0, \zeta_T), \quad (31)$$

with $\mathcal{F} : \mathbb{R}^{m+n} \rightarrow \mathbb{R}^n$, $\mathcal{G} : \mathbb{R}^{m+n} \rightarrow \mathbb{R}^{n_G}$, and $\mathcal{I} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{n_I}$. Let (ζ^0, α^0) be a solution. We call linearized system at point (ζ^0, α^0) the following DAE in the variables $\bar{\zeta}$ and $\bar{\alpha}$:

$$\dot{\bar{\zeta}}_t = \text{Lin } \mathcal{F} |_{(\zeta_t^0, \alpha_t^0)} (\bar{\zeta}_t, \bar{\alpha}_t), \quad (32)$$

$$0 = \text{Lin } \mathcal{G} |_{(\zeta_t^0, \alpha_t^0)} (\bar{\zeta}_t, \bar{\alpha}_t), \quad (33)$$

$$0 = \text{Lin } \mathcal{I} |_{(\zeta_0^0, \zeta_T^0)} (\bar{\zeta}_0, \bar{\zeta}_T), \quad (34)$$

where

$$\text{Lin } \mathcal{F} |_{(\zeta_t^0, \alpha_t^0)} (\bar{\zeta}_t, \bar{\alpha}_t) := \mathcal{F}'(\zeta_t^0, \alpha_t^0)(\bar{\zeta}_t, \bar{\alpha}_t), \quad (35)$$

and the analogous definitions for $\text{Lin } \mathcal{G}$ and $\text{Lin } \mathcal{H}$.

The technical result below will simplify the computation of the linearization of (OS). Its proof is immediate.

Lemma 4.2 (Commutation of linearization and differentiation). *Given \mathcal{G} and \mathcal{F} as in the previous definition, it holds:*

$$\frac{d}{dt} \text{Lin } \mathcal{G} = \text{Lin } \frac{d}{dt} \mathcal{G}, \quad \frac{d}{dt} \text{Lin } \mathcal{F} = \text{Lin } \frac{d}{dt} \mathcal{F}. \quad (36)$$

4.2 Linearized optimality system

In the sequel, whenever the argument of functions A, B, B_1 , etc. is omitted, assume that they are evaluated at the reference trajectory \hat{w} and at its unique multiplier $\hat{\lambda}$. Set

$$C := H_{ux}, \quad Q := H_{xx}. \quad (37)$$

The linearization of system (OS) at point $(\hat{x}, \hat{u}, \hat{\lambda})$ consists of the linearized state equation

$$\dot{z}_t = A_t z_t + B_t v_t, \quad t \in [0, T], \quad (38)$$

with initial-final conditions

$$0 = D\eta(\hat{x}_0, \hat{x}_T)(z_0, z_T), \quad (39)$$

the linearized costate equation

$$-\dot{q}_t = q_t A_t + z_t^\top Q_t + v_t^\top C_t, \quad \text{a.e. on } (0, T), \quad (40)$$

with initial-final conditions

$$q_0 = - \left[z_0^\top D_{x_0}^2 \ell + z_T^\top D_{x_0 x_T}^2 \ell + \sum_{j=1}^{d_\eta} \bar{\beta}_j D_{x_0} \eta_j \right]_{(\hat{x}_0, \hat{x}_T)}, \quad (41)$$

$$q_T = \left[z_T^\top D_{x_T}^2 \ell + z_0^\top D_{x_0 x_T}^2 \ell + \sum_{j=1}^{d_\eta} \bar{\beta}_j D_{x_T} \eta_j \right]_{(\hat{x}_0, \hat{x}_T)}, \quad (42)$$

and the algebraic equations

$$0 = \text{Lin } \ddot{\Phi} = -\frac{d^2}{dt^2}(qB + Cz), \quad \text{a.e. on } [0, T], \quad (43)$$

$$0 = \text{Lin } \Phi_T = q_T B_T + C_T z_T, \quad (44)$$

$$0 = \text{Lin } \dot{\Phi}_0 = -\frac{d}{dt}(qB + Cz)_{t=0}, \quad (45)$$

where we used equation (19) and commutation property of Lemma 4.2. There is no need to detail the derivatives in (43) and (45) since we will not make use of them later. Observe that (43)-(45) and Lemma 4.2 yield:

$$0 = \text{Lin } \Phi_t = q_t B_t + z_t^\top C_t^\top, \quad \text{on } [0, T]. \quad (46)$$

Note that equation (46) holds everywhere on $[0, T]$ since all the involved functions are continuous in time.

Notation: denote by (LS) the set of equations (38)-(45).

Once we have computed the linearized system, we can write the derivative of \mathcal{S} in the direction $\bar{v} := (z_0, q_0, \bar{\beta})$ as follows:

$$\mathcal{S}'(\hat{v})\bar{v} = \begin{pmatrix} D\eta(\hat{x}_0, \hat{x}_T)(z_0, z_T) \\ q_0 + \left[z_0^\top D_{x_0}^2 \ell + z_T^\top D_{x_0 x_T}^2 \ell + \sum_{j=1}^{d_\eta} \bar{\beta}_j D_{x_0} \eta_j \right]_{(\hat{x}_0, \hat{x}_T)} \\ q_T - \left[z_T^\top D_{x_T}^2 \ell + z_0^\top D_{x_0 x_T}^2 \ell + \sum_{j=1}^{d_\eta} \bar{\beta}_j D_{x_T} \eta_j \right]_{(\hat{x}_0, \hat{x}_T)} \\ q_T B_T + z_T^\top C_T \\ q_0 B_{1,0} \end{pmatrix}, \quad (47)$$

where (v, z, q) is the solution of (38), (40), (43) associated to the initial condition (z_0, q_0) and the multiplier $\bar{\beta}$. Thus, $\mathcal{S}'(\hat{v})$ is one-to-one if the only solution of (38)-(40), (43) with the initial conditions $z_0 = 0$, $q_0 = 0$ and with $\bar{\beta} = 0$ is $(v, z, q) = 0$.

5 Second order optimality conditions

We start this section by recalling a set of second order necessary and sufficient conditions. Afterwards we give the statement of the sufficient condition for the well-posedness of the shooting algorithm, that is the main result of this article.

Let Q and C be given in (37), and define the quadratic mapping on the space \mathcal{W} by

$$\Omega(z, v) := \frac{1}{2}D^2\ell(z_0, z_T)^2 + \frac{1}{2} \int_0^T [z^\top Qz + 2v^\top Cz] dt. \quad (48)$$

It is a well-known result that for each $(z, v) \in \mathcal{W}$,

$$D^2\mathcal{L}(z, v)^2 = \Omega(z, v). \quad (49)$$

Recall the classical second order necessary condition for optimality that states that the second variation of the Lagrangian function is non-negative over the cone of critical directions. In our case, the *critical cone* is given by

$$\mathcal{C} := \{(z, v) \in \mathcal{W} : (38)-(39) \text{ hold}\}, \quad (50)$$

and the second order optimality condition is as follows:

Theorem 5.1 (Second order necessary optimality condition). *If \hat{w} is a weak minimum of (P) then*

$$\Omega(z, v) \geq 0, \quad \text{on } \mathcal{C}. \quad (51)$$

A proof of previous theorem can be found in Levitin, Milyutin and Osolovskii [25].

Recall the definition of normal extremal in Section 2, and the following necessary condition due to Goh [19], that is a consequence of Theorem 5.1.

Theorem 5.2 (Goh's Necessary Condition). *If \hat{w} is a normal weak minimum of (P) then*

$$CB \text{ is symmetric.} \quad (52)$$

Next we recall a result due to Dmitruk [11], stated in terms of the coercivity of Ω in a transformed space of variables. Let us give the details of the involved transformation and the transformed second variation. Given $(z, v) \in \mathcal{W}$, define

$$y_t := \int_0^t v_s ds, \quad (53)$$

$$\xi_t := z_t - B(\hat{x}_t)y_t. \quad (54)$$

This change of variables, first introduced by Goh [20], can be done in any linear system of differential equations, and it is often called *Goh's transformation*.

We aim to perform Goh's transformation in (48). To this end consider the spaces $\mathcal{U}_2 := L_2(0, T; \mathbb{R}^m)$ and $\mathcal{X}_2 := W_2^1(0, T; \mathbb{R}^n)$, the $m \times n$ -matrix

$$M := B^\top Q - \dot{C} - CA, \quad (55)$$

the $m \times m$ -matrix

$$R := B^\top QB - CB_1 - (CB_1)^\top - \frac{d}{dt}(CB), \quad (56)$$

the function $g : \mathbb{R}^{2n+m} \rightarrow \mathbb{R}$ defined by

$$g(\zeta_0, \zeta_T, h) := D^2\ell(\zeta_0, \zeta_T + B_T h)^2 + h^\top C_T(2\zeta_T + B_T h), \quad (57)$$

and the quadratic mapping

$$\begin{aligned} \bar{\Omega} : \mathcal{X}_2 \times \mathcal{U}_2 \times \mathbb{R}^m &\rightarrow \mathbb{R} \\ (\xi, y, h) &\mapsto \frac{1}{2}g(\xi_0, \xi_T, h) + \frac{1}{2} \int_0^T \{\xi^\top Q \xi + 2y^\top M \xi + y^\top R y\} dt. \end{aligned} \quad (58)$$

Remark 5.3. Observe that R in (56) is symmetric since (52) holds.

Integrating by parts in (48) the terms containing v , and replacing z by its expression in (54) yields

$$\Omega(z, v) = \bar{\Omega}(\xi, y, y_T), \quad (59)$$

whenever $(z, v) \in \mathcal{W}$ and $(\xi, y, y_T) \in \mathcal{X} \times \mathcal{Y} \times \mathbb{R}^m$ satisfy (53)-(54). Set for each $(\xi_0, y, h) \in \mathbb{R}^n \times \mathcal{U}_2 \times \mathbb{R}^m$, the order:

$$\gamma(\xi_0, y, h) := |\xi_0|^2 + \int_0^T y_t^2 dt + |h|^2. \quad (60)$$

An element $(\delta x, v) \in \mathcal{W}$ is termed *feasible variation* for \hat{w} if $(\hat{x} + \delta x, \hat{u} + v)$ satisfies (2) and (3).

Definition 5.4. We say that \hat{w} satisfies γ -quadratic growth condition in the weak sense if there exists $\rho > 0$ such that, for every sequence of feasible variations $\{(\delta x^k, v^k)\}$ with $\{v^k\}$ converging to 0 in \mathcal{U} ,

$$J(\hat{u} + v^k) - J(\hat{u}) \geq \rho \gamma(\xi_0^k, y^k, y_T^k), \quad (61)$$

holds for big enough k , where $y_t^k := \int_0^t v_s^k ds$, and ξ is given by (54).

Observe that if $(z, v) \in \mathcal{W}$ satisfies (38)-(39), then $(\xi, y, h := y_T)$ given by (53)-(54) verifies

$$\dot{\xi} = A\xi + B_1 y, \quad (62)$$

$$D\eta(\hat{x}_0, \hat{x}_T)(\xi_0, \xi_T + B_T h) = 0. \quad (63)$$

Set the *transformed critical cone*:

$$\mathcal{P}_2 := \{(\xi, y, h) \in \mathcal{X}_2 \times \mathcal{U}_2 \times \mathbb{R}^m : (62)-(63) \text{ hold}\}. \quad (64)$$

The following is an immediate consequence of the sufficient condition established in Dmitruk [11] (or [12, Theorem 3.1]):

Theorem 5.5. The trajectory \hat{w} is a weak minimum of (P) satisfying γ -quadratic growth condition in the weak sense if and only if (52) holds and there exists $\rho > 0$ such that

$$\bar{\Omega}(\xi, y, h) \geq \rho \gamma(\xi_0, y, h), \quad \text{on } \mathcal{P}_2. \quad (65)$$

The result presented in [11] applies to a more general case having finitely many equalities and inequalities constraints on the initial and final state, and a set of multipliers consisting possibly of more than one element. In that case, condition (65) changes to a maximum on the subset of multipliers satisfying both (52) and $R \succeq 0$ on $[0, T]$.

Theorem 5.6 (Well-posedness in the free control case). *If \hat{w} is a weak minimum of (P) satisfying (65) then the shooting algorithm is well-posed in some neighborhood of \hat{w} . Furthermore, the approximating sequence (ν^k) defined by (27) converges quadratically to $\hat{\nu}$.*

We present the proof in the end of Section 7.

Remark 5.7. *It is interesting to observe that condition (65) is a quite weak assumption in the sense that: it is necessary for γ -quadratic growth and the corresponding relaxed condition (51) holds for every weak minimum.*

6 Corresponding LQ problem

In this section we present a linear-quadratic control problem (LQ) in the variables (ξ, y, h) having $\bar{\Omega}$ (defined in (58)) as cost functional. Afterwards we note that condition (65) yields the strong convexity of the pre-Hamiltonian of (LQ) and hence the uniqueness of the optimal solution. Furthermore, the unique optimal solution will be characterized by its first order optimality system, i.e., by the Pontryagin maximum principle. Finally we present a one-to-one linear mapping that transforms each solution of (LS) (introduced in section 4.2) into a solution of this new optimality system. Theorem 5.6 will follow.

Let us consider the linear-quadratic problem (LQ) given by:

$$\bar{\Omega}(\xi, y, h_T) \rightarrow \min, \quad (66)$$

$$(62)-(63), \quad (67)$$

$$\dot{h} = 0, \quad h_0 \text{ free.} \quad (68)$$

Here y is the control, ξ and h are the state variables. Denote by χ and χ_h the costate variables corresponding to ξ and h , respectively; and by ρ_0^{LQ} and β^{LQ} the multipliers associated to the cost function (66) and the initial-final state constraint (63), respectively. Put λ^{LQ} for the element $(\chi, \chi_h, \rho_0^{LQ}, \beta^{LQ})$. The pre-Hamiltonian for (LQ) is:

$$\mathcal{H}[\lambda^{LQ}](\xi, y) := \chi(A\xi + B_1y) + \frac{1}{2}(\xi^\top Q\xi + 2y^\top M\xi + y^\top Ry). \quad (69)$$

Observe that \mathcal{H} does not depend on h since it has zero dynamics and does not appear in the running cost. The initial-final Lagrangian is

$$\ell^{LQ}[\lambda^{LQ}](\xi_0, \xi_T, h_T) := \rho_0^{LQ} \frac{1}{2} g(\xi_0, \xi_T, h_T) + \sum_{j=1}^{d_\eta} \beta_j^{LQ} D\eta_j(\xi_0, \xi_T + B_T h_T). \quad (70)$$

The costate equation for χ is:

$$-\dot{\chi}_t = D_\xi \mathcal{H}[\lambda^{LQ}] = \chi A + \xi^\top Q + y^\top M, \quad (71)$$

with the boundary conditions:

$$\begin{aligned} \chi_0 &= -D_{\xi_0} \ell^{LQ}[\lambda^{LQ}] \\ &= -\rho_0^{LQ} \left[\xi_0^\top D_{x_0}^2 \ell + (\xi_T + B_T h)^\top D_{x_0 x_T}^2 \ell \right] - \sum_{j=1}^{d_\eta} \beta_j^{LQ} D_{x_0} \eta_j, \end{aligned} \quad (72)$$

$$\begin{aligned}
\chi_T &= D_{\xi_T} \ell^{LQ}[\lambda^{LQ}] \\
&= \rho_0^{LQ} \left[\xi_0^\top D_{x_0 x_T}^2 \ell + (\xi_T + B_T h)^\top D_{x_T^2}^2 \ell \right] + h^\top C_T + \sum_{j=1}^{d_\eta} \beta_j^{LQ} D_{x_T} \eta_j.
\end{aligned} \tag{73}$$

For costate variable χ_h we get the equation

$$-\dot{\chi}_h = 0, \tag{74}$$

$$\chi_{h,0} = 0, \tag{75}$$

$$\chi_{h,T} = D_h \ell^{LQ}[\lambda^{LQ}]. \tag{76}$$

Hence, $\chi_h \equiv 0$ and thus (76) yields

$$0 = \rho_0^{LQ} \left[\xi_0^\top D_{x_0 x_T}^2 \ell B_T + (\xi_T + B_T h)^\top (D_{x_T^2}^2 \ell B_T + C_T^\top) \right] + \sum_{j=1}^{d_\eta} \beta_j^{LQ} D_{x_T} \eta_j B_T. \tag{77}$$

The **stationarity with respect to the new control** y implies

$$0 = D_y \mathcal{H} = \chi B_1 + \xi^\top M^\top + y^\top R. \tag{78}$$

Notation: Denote by (LQS) the set of equations consisting of (62)-(68), (71)-(73), (77) and (78), and observe that (LQS) is an **optimality system** of problem (66)-(68).

Note that condition (65) is equivalent to the strong convexity of \mathcal{H} on the set of feasible solutions for problem (66)-(68). If \mathcal{H} is strongly convex, its unique critical point is a strict global minimum and it is characterized by the first optimality system (LQS).

7 The transformation

In this section we show how to transform a solution of (LS) into a solution of (LQS) via a one-to-one linear mapping. Given $(z, v, q, \bar{\beta}) \in \mathcal{X} \times \mathcal{U} \times \mathcal{X}_* \times \mathbb{R}^{d_\eta, *}$, define

$$\begin{aligned}
y_t &:= \int_0^t v_s ds, \quad \xi := z - B y, \quad \chi := q + y^\top C, \quad \chi_h := 0, \quad h := y_T, \\
\rho_0^{LQ} &:= 1, \quad \beta_j^{LQ} := \bar{\beta}_j.
\end{aligned} \tag{79}$$

The next lemma shows that the point $(\xi, y, h, \chi, \chi_h, \rho_0^{LQ}, \beta^{LQ})$ is solution of (LQS) provided that $(z, v, q, \bar{\beta})$ is solution of (LS).

Lemma 7.1. *The one-to-one linear mapping defined by (79) converts each solution of (LS) into a solution of (LQS).*

Proof. Let $(z, v, q, \bar{\beta})$ be a solution of (LS), and set $(\xi, y, \chi, \rho_0^{LQ}, \beta^{LQ})$ by (79).

Part I. We shall prove that $(\xi, y, \chi, \rho_0^{LQ}, \beta^{LQ})$ satisfies conditions (62) and (63). Equation (62) follows differentiating expression of ξ in (79), and equation (63) follows from (39).

Part II. We shall prove that $(\xi, y, \chi, \rho_0^{LQ}, \beta^{LQ})$ verifies (71)-(73) and (77). Differentiate χ in (79), use equations (40) and (79), recall definition of M in (55)

and obtain:

$$\begin{aligned}
-\dot{\chi} &= -\dot{q} - v^\top C - y^\top \dot{C} \\
&= qA + z^\top Q - y^\top \dot{C} \\
&= \chi A + \xi^\top Q + y^\top (-CA + B^\top Q - \dot{C}) \\
&= \chi A + \xi^\top Q + y^\top M.
\end{aligned} \tag{80}$$

Hence (71) holds. Equations (72) and (73) follow from (41) and (42). Combine (42) and (44) to get

$$\begin{aligned}
0 &= q_T B_T + z_T^\top C_T^\top \\
&= \left[z_T^\top D_{x_T}^2 \ell + z_0^\top D_{x_0 x_T}^2 \ell + \sum_{j=1}^{d_\eta} \bar{\beta}_j D_{x_T} \eta_j \right]_{(\hat{x}_0, \hat{x}_T)} B_T + z_T^\top C_T^\top.
\end{aligned} \tag{81}$$

Performing transformation (79) in the previous equation yields (77).

Part III. We shall prove that (78) holds. Differentiating (46) we get

$$0 = \frac{d}{dt} \text{Lin } \Phi = \frac{d}{dt} (qB + z^\top C^\top). \tag{82}$$

Consequently, by (38) and (40),

$$0 = -(qA + z^\top Q + v^\top C)B + q\dot{B} + (z^\top A^\top + v^\top B^\top)C^\top + z^\top \dot{C}^\top, \tag{83}$$

where the coefficient of v vanishes by condition (52). Recall (18) and (55). Performing transformation (79) and regrouping the terms we get from (83),

$$0 = -\chi B_1 - \xi^\top M^\top + y^\top (CB_1 - B^\top QB + B^\top A^\top C^\top + B^\top \dot{C}^\top). \tag{84}$$

Equation (78) follows from (56) and condition (52).

Parts I, II and III show that $(\xi, y, \chi, \rho_0^{LQ}, \beta^{LQ})$ is a solution of (LQS), and hence the result follows. \square

Remark 7.2. Observe that the unique assumption we needed in previous proof was the symmetry condition (52) that follows from the weak optimality of \hat{w} .

of Theorem 5.6. We shall prove the first statement. Let $(z, v, q, \bar{\beta})$ be a solution of (LS), and let $(\xi, y, \chi, \chi_h, \rho_0^{LQ}, \beta^{LQ})$ be defined by (79), that we know by Lemma 7.1 is solution of (LQS). Since (65) holds, the cost function of problem (66)-(68) is strongly convex and thus the unique solution of its optimality system (LQS) is 0. Hence $(\xi, y, \chi, \chi_h, \rho_0^{LQ}, \beta^{LQ}) = 0$ and thus $(z, v, q, \bar{\beta}) = 0$. Conclude that the unique solution of (LQ) is 0. This implies the injectivity of \mathcal{S}' around a neighborhood of \hat{v} , and hence the result follows.

The quadratic convergence follows from $\mathcal{S}(\hat{v}) = 0$, i.e., the residual is zero. See Fletcher [15] or Bonnans [5] for a proof of this quadratic convergence. \square

8 Control constrained case

In this section we add the following bounds to the control variables

$$0 \leq u_{i,t} \leq 1, \quad \text{for a.a. } t \in [0, T], \text{ for } i = 1, \dots, m. \tag{85}$$

Denote with (CP) the problem given by (1)-(3) and (85). We study a solution $\hat{w} \in \mathcal{W}$, that is a *Pontryagin minimum* of (CP), i.e., for any positive N there

exists $\varepsilon_N > 0$ such that \hat{w} is a minimum in the set of feasible trajectories $w = (x, u) \in \mathcal{W}$ satisfying

$$\|x - \hat{x}\|_\infty < \varepsilon_N, \|u - \hat{u}\|_1 < \varepsilon_N, \|u - \hat{u}\|_\infty < N.$$

Given $i = 1, \dots, m$, we say that \hat{u}_i has a *bang arc* in $(a, b) \subset (0, T)$ if $\hat{u}_{i,t} = 0$ a.e. on (a, b) or $\hat{u}_{i,t} = 1$ a.e. on (a, b) , and it has a *singular arc* if $0 < \hat{u}_{i,t} < 1$ a.e. on (a, b) .

Assumption 8.1. *Each component \hat{u}_i is a finite concatenation of bang and singular arcs.*

A time $t \in (0, T)$ is called *switching time* if there exists an index $1 \leq i \leq m$ such that \hat{u}_i changes at time t from singular to bang, or vice versa, or from one bound in (85) to the other.

With the purpose of solving (CP) numerically we assume that the structure of the concatenation of bang and singular arcs of the optimal solution \hat{w} and an approximation of its switching times are known. This initial guess can be obtained, for instance, by solving the nonlinear problem resulting from the discretization of the optimality conditions or by a continuation method. See Betts [3] or Biegler [4] for a detailed survey and description of numerical methods for nonlinear programming problems. For the continuation method the reader is referred to Martinon [27].

This section is organized as follows. From (CP) and the known structure of \hat{u} and its switching times we create a new problem that we denote by (TP). Afterwards we prove that we can transform \hat{w} into a weak solution \hat{W} of (TP). Finally we conclude that if \hat{W} satisfies the coercivity condition (65), then the shooting method for problem (TP) is well-posed and converges quadratically provided that we start from a good initialization. In practice, the procedure will be as follows: obtain somehow the structure of the optimal solution of (CP), create problem (TP), solve (TP) numerically obtaining \hat{W} , and finally transform \hat{W} to find \hat{w} .

Next we present the transformed problem.

Assumption 8.2. *Assume that each time a control \hat{u}_i passes from bang to singular or vice versa, there is a discontinuity of first kind, i.e., a finite jump.*

By Assumption 8.1 the set of switching times is finite. Consider the partition of $[0, T]$ induced by the switching times:

$$\{0 =: \hat{T}_0 < \hat{T}_1 < \dots < \hat{T}_{N-1} < \hat{T}_N := T\}. \quad (86)$$

Set $\hat{I}_k := (\hat{T}_{k-1}, \hat{T}_k)$, and define for $k = 1, \dots, N$,

$$S_k := \{1 \leq i \leq m : \hat{u}_i \text{ is singular on } \hat{I}_k\}, \quad (87)$$

$$E_k := \{1 \leq i \leq m : \hat{u}_i = 0 \text{ a.e. on } \hat{I}_k\}, \quad (88)$$

$$N_k := \{1 \leq i \leq m : \hat{u}_i = 1 \text{ a.e. on } \hat{I}_k\}. \quad (89)$$

It could happen $S_k = \emptyset$, $E_k = \emptyset$ or $N_k = \emptyset$.

Assumption 8.3. For each $k = 1, \dots, N$, denote with u_{S_k} the vector with components u_i with $i \in S_k$. Assume that the strengthened generalized Legendre-Clebsch (LC) condition holds on \hat{I}_k , i.e.,

$$-\frac{\partial}{\partial u_{S_k}} \ddot{H}_{u_{S_k}} \succ 0, \quad \text{on } \hat{I}_k. \quad (90)$$

This implies that the singular arcs are of order 1. Thus u_{S_k} can be retrieved from equation

$$\ddot{H}_{u_{S_k}} = 0. \quad (91)$$

Remark 8.4. Note that (90) is a consequence of the sufficient condition (65).

Since the expression obtained from (91) involves only the state variable \hat{x} and the corresponding adjoint state \hat{p} , we deduce that u_{S_k} is continuous on \hat{I}_k . As the components u_i with $i \notin S_k$ are either identically 1 or 0, we conclude that

$$u \text{ is continuous on } \hat{I}_k. \quad (92)$$

Actually, Assumptions 8.2 and 8.3 together are quite natural. This can be justified by the work due to McDanell and Powers [31], where they presented some necessary conditions for the discontinuity of \hat{u}_i involving the generalized LC condition.

By the Assumption 8.2 and condition (92) (derived from Assumption 8.3) we get that there exists $\rho > 0$ such that for each $k = 1, \dots, N$ and $i \in S_k$,

$$\rho < \hat{u}_{i,t} < 1 - \rho, \quad \text{a.e. on } \hat{I}_k. \quad (93)$$

Next we present a new control problem obtained in the following way: for each $k = 1, \dots, N$, we perform the change of time variable that converts the interval $(\hat{T}_{k-1}, \hat{T}_k)$ into $(0, 1)$, we fix the bang control variables to their bounds and we associate a free control variable to each index in S_k . More precisely, consider for $k = 1, \dots, N$ the control variables $u_i^k \in L_\infty(0, 1; \mathbb{R})$, with $i \in S_k$, and the state variables $x^k \in W_\infty^1(0, 1; \mathbb{R}^n)$. Let the constants $T_k \in \mathbb{R}$, for $k = 1, \dots, N - 1$, which will be considered as state variable of zero-dynamics. Set $T_0 := 0$, $T_N := T$ and define the problem

$$\varphi_0(x_0^1, x_1^N) \rightarrow \min, \quad (94)$$

$$\dot{x}^k = (T_k - T_{k-1}) \left(\sum_{i \in N_k \cup \{0\}} f_i(x^k) + \sum_{i \in S_k} u_i^k f_i(x^k) \right), \quad k = 1, \dots, N, \quad (95)$$

$$\dot{T}_k = 0, \quad k = 1, \dots, N - 1, \quad (96)$$

$$\eta(x_0^1, x_1^N) = 0, \quad (97)$$

$$x_1^k = x_0^{k+1}, \quad k = 1, \dots, N - 1. \quad (98)$$

Denote by (TP) the problem consisting of equations (94)-(98). The link between the original problem (CP) and the transformed one (TP) is given in Lemma 8.5 below. Set for each $k = 1, \dots, N$:

$$\hat{x}_s^k := \hat{x}(\hat{T}_{k-1} + (\hat{T}_k - \hat{T}_{k-1})s), \quad (99)$$

$$\hat{u}_{i,s}^k := \hat{u}_i(\hat{T}_{k-1} + (\hat{T}_k - \hat{T}_{k-1})s), \quad \text{for } i \in S_k. \quad (100)$$

Set

$$\hat{W} := ((\hat{x}^k)_{k=1}^N, (\hat{u}_i^k)_{k=1, i \in S_k}^N, (\hat{T}_k)_{k=1}^{N-1}). \quad (101)$$

Lemma 8.5. *The point \hat{W} is a weak solution of (TP).*

Proof. The idea of the proof is deriving the weak optimality of \hat{W} from the Pontryagin optimality of \hat{w} and condition (93). Since \hat{w} is a Pontryagin minimum for (CP), there exists $\varepsilon > 0$, such that \hat{w} is a minimum in the set of feasible trajectories $w = (x, u)$ satisfying

$$\|x - \hat{x}\|_\infty < \varepsilon, \quad \|u - \hat{u}\|_1 < \varepsilon, \quad \|u - \hat{u}\|_\infty < 1. \quad (102)$$

Consider $\bar{\delta}, \bar{\varepsilon} > 0$, and a feasible solution $((x^k), (u_i^k), (T_k))$ for (TP) such that

$$|T_k - \hat{T}_k| \leq \bar{\delta}, \quad \|u_i^k - \hat{u}_i^k\|_\infty < \bar{\varepsilon}, \quad \text{for all } k = 1, \dots, N. \quad (103)$$

We shall relate ε in (102) with $\bar{\delta}$ and $\bar{\varepsilon}$ in (103). Let $k = 1, \dots, N$. Denote $I_k := (T_{k-1}, T_k)$, and define for each $i = 1, \dots, m$:

$$u_{i,t} := \begin{cases} 0, & \text{if } t \in I_k \text{ and } i \in E_k, \\ u_i^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right), & \text{if } t \in I_k \text{ and } i \in S_k, \\ 1, & \text{if } t \in I_k \text{ and } i \in N_k. \end{cases} \quad (104)$$

Let x be the solution of (2) corresponding to u and having $x(0) = x_0^1$. We shall prove that (x, u) is feasible for the original problem (CP). Observe that condition (98) implies that $x_t = x^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right)$ when $t \in I_k$, and thus $x_1 = x_1^N$. It follows that (3) holds. We shall check condition (85). For $i \in E_k \cup N_k$, it follows from the definition in (104). Consider now $i \in S_k$. Since (93) holds, by (100) we get

$$\rho < \hat{u}_{i,s}^k < 1 - \rho, \quad \text{a.e. on } (0, 1). \quad (105)$$

Thus, by (103) and if $\bar{\varepsilon} < \rho$, we get $0 < u_{i,s}^k < 1$ a.e. on $(0, 1)$. This yields

$$0 < u_{i,t} < 1, \quad \text{a.e. on } I_k, \quad (106)$$

and thus the feasibility of (x, u) for (CP).

Let us look for an estimate of $\|u - \hat{u}\|_1$. For $k = 1, \dots, N$ and $i \in S_k$,

$$\int_{I_k \cap \hat{I}_k} |u_{i,t} - \hat{u}_{i,t}| dt \leq \int_{I_k \cap \hat{I}_k} \left| u_i^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right) - \hat{u}_i^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right) \right| dt \\ + \int_{I_k \cap \hat{I}_k} \left| \hat{u}_i^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right) - \hat{u}_i^k \left(\frac{t - \hat{T}_{k-1}}{\hat{T}_k - \hat{T}_{k-1}} \right) \right| dt. \quad (107)$$

Note that by Assumption 8.2 and condition (92), each \hat{u}_i^k is uniformly continuous on \hat{I}_k , and thus there exists $\theta_{ki} > 0$ such that if $|s - s'| < \theta_{ki}$ then $|\hat{u}_{i,s}^k - \hat{u}_{i,s'}^k| < \bar{\varepsilon}$. Set $\bar{\theta} := \min \theta_{ki} > 0$. Consider then $\bar{\delta}$ such that if $|T_k - \hat{T}_k| < \bar{\delta}$, then $\left| \frac{t - T_{k-1}}{T_k - T_{k-1}} - \frac{t - \hat{T}_{k-1}}{\hat{T}_k - \hat{T}_{k-1}} \right| < \bar{\theta}$. From (103) and (107) we get

$$\int_{I_k \cap \hat{I}_k} |u_{i,t} - \hat{u}_{i,t}| dt < 2\bar{\varepsilon} \text{meas}(I_k \cap \hat{I}_k). \quad (108)$$

Assume, w.l.g., that $T_k < \hat{T}_k$ and note that

$$\int_{T_k}^{\hat{T}_k} |u_{i,t} - \hat{u}_{i,t}| dt \leq \int_{T_k}^{\hat{T}_k} \left| u_i^k \left(\frac{t - T_{k-1}}{T_k - T_{k-1}} \right) - \hat{u}_i^k \left(\frac{t - \hat{T}_{k-1}}{\hat{T}_k - \hat{T}_{k-1}} \right) \right| dt < \bar{\delta} \bar{\varepsilon}, \quad (109)$$

where we used (103) in the last inequality. From (108) and (109) we get $\|u_i - \hat{u}_i\|_1 < \bar{\varepsilon}(2T + (N-1)\bar{\delta})$. Thus $\|u - \hat{u}\|_1 < \varepsilon$ if

$$\bar{\varepsilon}(2T + (N-1)\bar{\delta}) < \varepsilon/m. \quad (110)$$

We conclude from (102) that $((x^k), (u_i^k), (T_k))$ is a minimum on the set of feasible points satisfying (103) and (110). Thus \hat{W} is a weak solution of (TP), as it was to be proved. \square

Remark 8.6. *It can be shown that \hat{W} is a Pontryagin minimum of problem (TP) with the additional constraints $0 \leq u_i^k \leq 1$.*

Let us look for the shooting function associated to (TP). Observe that its pre-Hamiltonian is

$$\tilde{H} := \sum_{k=1}^N (T_k - T_{k-1}) H^k, \quad (111)$$

where, denoting with p^k the costate variable associated to x^k ,

$$H^k := p^k \left(\sum_{i \in N_k \cup \{0\}} f_i(x^k) + \sum_{i \in S_k} u_i^k f_i(x^k) \right). \quad (112)$$

The initial-final Lagrangian is

$$\tilde{\ell} := \alpha_0 \varphi_0(x_0^1, x_1^N) + \sum_{j=1}^{d_\eta} \beta_j \eta_j(x_0^1, x_1^N) + \sum_{k=1}^{N-1} \theta_k (x_1^k - x_0^{k+1}). \quad (113)$$

The costate equation for p^k is given by

$$\dot{p}^k = -(T_k - T_{k-1}) D_{x^k} H^k, \quad (114)$$

with initial-final conditions

$$p_0^1 = -D_{x_0^1} \tilde{\ell} = -\alpha_0 D_{x_0^1} \varphi_0 - \sum_{j=1}^{d_\eta} \beta_j D_{x_0^1} \eta_j, \quad (115)$$

$$\begin{aligned} p_1^k &= \theta^k, & \text{for } k = 1, \dots, N-1, \\ p_0^k &= \theta^{k-1}, & \text{for } k = 2, \dots, N, \end{aligned} \quad (116)$$

$$p_1^N = D_{x_1^N} \tilde{\ell} = \alpha_0 D_{x_1^N} \varphi_0 + \sum_{j=1}^{d_\eta} \beta_j D_{x_1^N} \eta_j, \quad (117)$$

For the costate variables p^{T_k} associated with T_k we get the equations

$$\dot{p}^{T_k} = -H^k + H^{k+1}, \quad p_0^{T_k} = 0, \quad p_1^{T_k} = 0. \quad (118)$$

Remark 8.7. *We can sum up these three conditions integrating the first one and obtaining $\int_0^1 (H^{k+1} - H^k) dt = 0$, and hence, since H^k is constant on the optimal trajectory, we get the equivalent condition*

$$H^k(1) = H^{k+1}(0), \quad \text{for } k = 1, \dots, N-1. \quad (119)$$

Observe that conditions (98) and (116) imply the continuity of the two functions obtained by concatenating the states and the costates, i.e., the continuity of X and P defined by

$$X_0 := x_0^1, \quad X_s := x^k(s - (k - 1)), \quad \text{for } s \in (k - 1, k], \quad k = 1, \dots, N, \quad (120)$$

$$P_0 := p_0^1, \quad P_s := p^k(s - (k - 1)), \quad \text{for } s \in (k - 1, k], \quad k = 1, \dots, N. \quad (121)$$

Thus, while iterating the shooting method, we can either include the conditions (98) and (116) in the definition of the shooting function or integrate the differential equations for x^k and p^k from the values x_1^{k-1} and p_1^{k-1} previously obtained. The latter option reduces the number of variables and hence the size of the problem, but is less stable. We shall present below the shooting function for the more stable case. For this end define the $n \times n$ -matrix

$$A^k := \sum_{i \in N_k \cup \{0\}} f'_i(\hat{x}^k) + \sum_{i \in S_k} \hat{u}_i^k f'_i(\hat{x}^k), \quad (122)$$

the $n \times |S_k|$ -matrix B^k with columns $f_i(\hat{x}^k)$ with $i \in S_k$, and

$$B_1^k := A^k B^k - \frac{d}{dt} B^k. \quad (123)$$

The resulting shooting function for (TP) is given by

$$\mathcal{S} : \mathbb{R}^{Nn+N-1} \times \mathbb{R}^{Nn+N-1+d_\eta,*} \rightarrow \mathbb{R}^{d_\eta+(N-1)n} \times \mathbb{R}^{(N+1)n+N-1+2\sum |N_k|,*},$$

$$((x_0^k), (T_k), (p_0^k), (p_0^{T_k}), \beta) =: \nu \mapsto \mathcal{S}(\nu) := \begin{pmatrix} \eta(x_0^1, x_1^N) \\ (x_1^k - x_0^{k+1})_{k=1, \dots, N-1} \\ p_0^1 + D_{x_0^1} \tilde{\ell}[\lambda](x_0^1, x_1^N) \\ (p_1^k - p_0^{k+1})_{k=1, \dots, N-1} \\ p_1^N - D_{x_1^N} \tilde{\ell}[\lambda](x_0^1, x_1^N) \\ (p_1^{T_k})_{k=1, \dots, N-1} \\ (p_1^k B^k(x_1^k))_{k=1, \dots, N} \\ (p_0^k B_1^k(x_0^k))_{k=1, \dots, N} \end{pmatrix}. \quad (124)$$

Given that problem (TP) has the same structure than problem (P) in section 2, i.e., they both have initial-final constraints and free control variable, we can apply Theorem 5.6 and obtain:

Theorem 8.8 (Well-posedness in the control constrained case). *Assume that \hat{w} is a Pontryagin minimum of (CP) such that \hat{W} defined in (101) satisfies condition (65) for problem (TP). Then the shooting algorithm for (TP) is well-posed around \hat{W} .*

Remark 8.9. *Once system (124) is obtained, observe that two numerical implementations can be done: one integrating each variable in the interval $[0, 1]$ and the other one, going back to the original interval $[0, T]$, as it is done in the numerical tests of Section 10 below. In the latter case, the sensibility with respect to the switching times is obtained from the derivative of the shooting function.*

Remark 8.10. *In view of Remark 8.7 note that we can remove the variables p^{T_k} from the formulation either imposing the condition (119) if we integrate in $[0, 1]$, or enforcing*

$$H(t_k+) = H(t_{k+1}-), \quad k = 1, \dots, N-1, \quad (125)$$

when the integration is on $[0, T]$.

Remark 8.11. *Let us note that for some problems, certain conditions in (124) are redundant. Consider, for instance, a solution having a bang-to-singular switching at time t_k . Then the condition $\Phi(t_k) = 0$, implied by the singularity of the arc, yields $\hat{p}f_i(\hat{x}(t_k)) = 0$. Thus, in H , the coefficients of the jumps vanish. Hence, $\Phi(t_k) = 0$ implies that H is continuous at t_k , and this can be translated, in view of (118), (119) and previous remark, that we do not need to impose $p_1^{T_k} = 0$.*

Remark 8.12 (Square Systems). *In some cases, the formulation (124) turns out to be square as it can be seen in the examples 1 and 3 of Section 10. Actually, our formulation yields a square system if and only if each singular arc is in the interior of $(0, T)$ and at each switching time only one control component switches. In this case we remove the condition of continuity of H at the bang-to-singular switchings to obtain a square system.*

Remark 8.13. *Consider a case containing a singular arc starting at $t = 0$ (or finishing at $t = T$). Here, we impose $\Phi = \dot{\Phi} = 0$ at the exit (or entry) time. Hence, we can notice that each singular arc of this type contributes to the shooting function with two equations and only one variable.*

9 Stability under data perturbation

In this section we investigate the stability of the optimal solution under data perturbation. Assume for this stability analysis that the shooting system of the studied problem is square. We gave a description of this situation in Remark 8.12 above. We shall prove that, under condition (65), the solution is stable under small perturbations of the data functions φ_0 , f_i and η .

9.1 Unconstrained control case

Consider then problem (P) presented in Section 2, and the family of problems depending on the real parameter μ given by:

$$\begin{aligned} \varphi_0^\mu(x_0, x_T) &\rightarrow \min, \\ \dot{x}_t &= \sum_{i=0}^m u_{i,t} f_i^\mu(x_t), \quad \text{for } t \in (0, T), \\ \eta^\mu(x_0, x_T) &= 0. \end{aligned} \quad (\text{P}_\mu)$$

Assume that $\varphi_0^\mu : \mathbb{R}^{2n+1} \rightarrow \mathbb{R}$ and $\eta^\mu : \mathbb{R}^{2n+1} \rightarrow \mathbb{R}^{d_\eta}$ are twice continuously differentiable in the variable (x_0, x_T) and continuously differentiable with respect to μ , and $f_i^\mu : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ is twice continuously differentiable with respect to x and continuously differentiable with respect to the parameter μ . In this formulation, problem (P_0) coincides with (P), i.e., $\varphi_0^0 = \varphi_0$, $f_i^0 = f_i$ for $i = 0, \dots, m$

and $\eta^0 = \eta$. Recall (65) in Theorem 5.5, and write the analogous condition for (P_μ) as follows:

$$\bar{\Omega}^\mu(\xi, y, h) \geq \rho\gamma(\xi_0, y, h), \quad \text{on } \mathcal{P}_2^\mu, \quad (126)$$

where $\bar{\Omega}^\mu$ and \mathcal{P}_2^μ are the second variation and critical cone associated to (P_μ) , respectively. Note that each (P_μ) defines a shooting function that we denote by \mathcal{S}^μ . Thus, we can write

$$\begin{aligned} \mathcal{S}^\mu : \mathbb{R}^M \times \mathbb{R} &\rightarrow \mathbb{R}^M, \\ (\nu, \mu) &\mapsto \mathcal{S}^\mu(\nu), \end{aligned} \quad (127)$$

where we indicate with M the dimension of the domain of \mathcal{S} . The following stability result will be established:

Theorem 9.1 (Stability of the optimal solution). *Assume that the shooting system generated by problem (P) is square and let \hat{w} be a solution satisfying the uniform positivity condition (65). Then there exists a neighborhood $\mathcal{J} \subset \mathbb{R}$ of 0, and a continuous differentiable mapping $\mu \mapsto w^\mu = (x^\mu, u^\mu)$, from \mathcal{J} to \mathcal{W} , where w^μ is a weak solution for (P_μ) . Furthermore, w^μ verifies the uniform positivity (126). Therefore, in view of Theorems 5.5 and 5.6, the quadratic growth in the weak sense holds, and the shooting algorithm for (P^μ) is well-posed.*

Let us start showing the following stability result for the family of shooting functions $\{\mathcal{S}^\mu\}$:

Lemma 9.2. *Assume the same hypotheses that in Theorem 9.1. Then there exists a neighborhood $\mathcal{I} \subset \mathbb{R}$ of 0 and a continuous differentiable mapping $\mu \mapsto \nu^\mu = (x_0^\mu, p_0^\mu, \beta^\mu)$, from \mathcal{I} to \mathbb{R}^M , such that $\mathcal{S}^\mu(\nu^\mu) = 0$. Furthermore, the solutions (x^μ, u^μ, p^μ) of (2)-(7)-(15) with initial condition (x_0^μ, p_0^μ) and associated multiplier β^μ provide a family of feasible trajectories $w^\mu := (x^\mu, u^\mu)$ verifying*

$$\|x^\mu - \hat{x}\|_\infty + \|u^\mu - \hat{u}\|_\infty + \|p^\mu - \hat{p}\|_\infty + |\beta^\mu - \hat{\beta}| = \mathcal{O}(\mu). \quad (128)$$

Proof. Since (65) holds, the well-posedness result in Theorem 5.6 yields the non-singularity of the square matrix $D_\nu \mathcal{S}^0(\hat{\nu})$. Hence, the Implicit Function Theorem is applicable and we can then guarantee the existence of a neighborhood $\mathcal{B} \subset \mathbb{R}^M$ of $\hat{\nu}$, a neighborhood $\mathcal{I} \subset \mathbb{R}$ of 0, and a continuously differentiable function $\Gamma : \mathcal{I} \rightarrow \mathcal{B}$ such that

$$\mathcal{S}^\mu(\Gamma(\mu)) = 0, \quad \text{for all } \mu \in \mathcal{I}. \quad (129)$$

Finally, write $\nu^\mu := \Gamma(\mu)$ and use the continuity of $D\Gamma$ on \mathcal{I} to get the first part of the statement.

The feasibility of w^μ holds since equation (129) is verified. Finally, the estimation (128) follows from the stability of the system of differential equation provided by the shooting method. \square

Once we obtained the existence of this w^μ feasible for (P^μ) , we may wonder whether it is locally optimal. For this aim, we shall investigate the stability of the sufficient condition (65). Denote by $\bar{\Omega}^\mu$ and \mathcal{P}_2^μ the quadratic mapping and critical cone related to (P^μ) , respectively. Given that all the functions involved in $\bar{\Omega}^\mu$ are continuously differentiable with respect to μ , the mapping $\bar{\Omega}^\mu$ itself is continuously differentiable with respect to μ . For the perturbed cone we get the following approximation result:

Lemma 9.3. *Assume the same hypotheses imposed in Theorem 9.1. Take $\mu \in \mathcal{I}$ and $(\xi^\mu, y^\mu, h^\mu) \in \mathcal{P}_2^\mu$. Then there exists $(\xi, y, h) \in \mathcal{P}_2$ such that*

$$|\xi_0^\mu - \xi_0| + \|y^\mu - y\|_2 + |h^\mu - h| = \mathcal{O}(\mu). \quad (130)$$

The definition below will be useful in the proof of previous Lemma.

Definition 9.4. *Define the function $\bar{\eta} : \mathcal{U} \times \mathbb{R}^n \rightarrow \mathbb{R}^{d_\eta}$, given by*

$$\bar{\eta}(u, x_0) := \eta(x_0, x_T), \quad (131)$$

where x is the solution of (2) associated to (u, x_0) .

of Lemma 9.3. We shall start by showing that Assumption 2.2 implies that $D\bar{\eta}(\hat{u}, \hat{x}_0)$ is onto. Suppose on the contrary that $D\bar{\eta}(\hat{u}, \hat{x}_0)$ is not onto. Hence, there exists $\beta \neq 0$ in \mathbb{R}^{d_η} such that $\sum_{j=1}^{d_\eta} \beta_j D\bar{\eta}_j(\hat{u}, \hat{x}_0) = 0$. Take $\alpha_0 := 0$ and $p := 0$, and observe that both $\lambda := (\alpha_0, \beta \cdot p)$ and $-\lambda$ are Pontryagin multipliers for \hat{w} . This contradicts normality condition 11, and hence the surjectivity of $D\bar{\eta}(\hat{u}, \hat{x}_0)$ follows.

Recall now the definition of the critical cone \mathcal{C} given in (50), and notice that we can rewrite it as

$$\mathcal{C} = \{(z, v) \in \mathcal{W} : \mathcal{G}(z, v) = 0\} = \text{Ker } \mathcal{G}, \quad (132)$$

with $\mathcal{G}(z, v) := D\eta(\hat{x}_0, \hat{x}_T)(z_0, z_T)$ being an onto linear application from \mathcal{W} to \mathbb{R}^{d_η} . In view of Goh's Transformation (53)-(54),

$$D\eta(\hat{x}_0, \hat{x}_T)(z_0, z_T) = D\eta(\hat{x}_0, \hat{x}_T)(\xi_0, \xi_T + B_T y_T), \quad (133)$$

for $(z, v) \in \mathcal{W}$ and (ξ, y) being its corresponding transformed direction. Thus, the cone \mathcal{P}_2 can be written as $\mathcal{P}_2 = \{\zeta \in \mathcal{H} : \mathcal{K}(\zeta) = 0\} = \text{Ker } \mathcal{K}$, with $\zeta := (\xi, y, h)$, $\mathcal{H} := \mathcal{X}_2 \times \mathcal{U}_2 \times \mathbb{R}^n$, and $\mathcal{K}(\zeta) := D\eta(\hat{x}_0, \hat{x}_T)(\xi_0, \xi_T + B_T h)$. Then $\mathcal{K} \in \mathcal{L}(\mathcal{H}, \mathbb{R}^{d_\eta})$ and it is surjective. Analogously,

$$\mathcal{P}_2^\mu = \{\zeta \in \mathcal{H} : \mathcal{K}^\mu(\zeta) = 0\} = \text{Ker } \mathcal{K}^\mu, \quad (134)$$

with

$$\|\mathcal{K}^\mu - \mathcal{K}\|_{\mathcal{L}(\mathcal{H}, \mathbb{R}^{d_\eta})} = \mathcal{O}(\mu). \quad (135)$$

Let us now prove the desired stability property. Take $\zeta^\mu \in \mathcal{P}_2^\mu = \text{Ker } \mathcal{K}^\mu$ having $\|\zeta^\mu\|_{\mathcal{H}}^\mu = 1$. Hence

$$\mathcal{K}(\zeta^\mu) = \mathcal{K}^\mu(\zeta^\mu) + (\mathcal{K} - \mathcal{K}^\mu)(\zeta^\mu), \quad (136)$$

and by estimation (135),

$$|\mathcal{K}(\zeta^\mu)| = \mathcal{O}(\mu). \quad (137)$$

Observe that, since $\mathcal{H} = \text{Ker } \mathcal{K} \oplus \text{Im } \mathcal{K}^\top$, there exists $\zeta^{\mu,*} \in \mathcal{H}^*$ such that

$$\zeta := \zeta^\mu + \mathcal{K}^\top(\zeta^{\mu,*}) \in \text{Ker } \mathcal{K}. \quad (138)$$

This yields $0 = \mathcal{K}(\zeta) = \mathcal{K}(\zeta^\mu) + \mathcal{K}\mathcal{K}^\top(\zeta^{\mu,*}) = (\mathcal{K} - \mathcal{K}^\mu)(\zeta^\mu) + \mathcal{K}\mathcal{K}^\top(\zeta^{\mu,*})$. Given that \mathcal{K} is onto, the operator $\mathcal{K}\mathcal{K}^\top$ is invertible and thus

$$\zeta^{\mu,*} = -(\mathcal{K}\mathcal{K}^\top)^{-1}(\mathcal{K} - \mathcal{K}^\mu)(\zeta^\mu). \quad (139)$$

The estimation (137) above implies $\|\zeta^{\mu,*}\|_{\mathcal{H}^*} = \mathcal{O}(\mu)$. It follows then from (138) that $\|\zeta^\mu - \zeta\|_{\mathcal{H}} = \mathcal{O}(\mu)$, and therefore, the desired result holds. \square

of Theorem 9.1. We shall begin by observing that Lemma 9.2 provides a neighborhood \mathcal{I} and a class of solutions $\{(x^\mu, u^\mu, p^\mu, \beta^\mu)\}_{\mu \in \mathcal{I}}$ satisfying (128). We shall prove that $w^\mu = (x^\mu, u^\mu)$ satisfies the sufficient condition (126) close to 0.

Suppose on the contrary that there exists a sequence of parameters $\mu_k \rightarrow 0$ and critical directions $(\xi^{\mu_k}, y^{\mu_k}, h^{\mu_k}) \in \mathcal{P}_2^{\mu_k}$ with $\gamma(\xi_0^{\mu_k}, y^{\mu_k}, h^{\mu_k}) = 1$, such that

$$\bar{\Omega}^{\mu_k}(\xi^{\mu_k}, y^{\mu_k}, h^{\mu_k}) \leq o(1). \quad (140)$$

Since $\bar{\Omega}^\mu$ is Lipschitz-continuous in μ , from previous inequality we get

$$\bar{\Omega}(\xi^{\mu_k}, y^{\mu_k}, h^{\mu_k}) \leq o(1). \quad (141)$$

In view of Lemma 9.3, there exists for each k , a direction $(\xi^k, y^k, h^k) \in \mathcal{P}_2$ satisfying

$$|\xi_0^k - \xi_0^{\mu_k}| + \|y^k - y^{\mu_k}\|_2 + |h^k - h^{\mu_k}| = \mathcal{O}(\mu_k). \quad (142)$$

Hence, by inequality (141) and given that \hat{w} satisfies (65),

$$\rho\gamma(\xi_0^k, y^k, h^k) \leq \bar{\Omega}(\xi^k, y^k, h^k) \leq o(1). \quad (143)$$

However, the left hand-side of this last inequality cannot go to 0 since (ξ_0^k, y^k, h^k) is close to $(\xi_0^{\mu_k}, y^{\mu_k}, h^{\mu_k})$ by estimation (142), and the elements of the latter sequence have unit norm. This leads to a contradiction. Hence, the result follows. \square

9.2 Control constrained case

In this paragraph we aim to investigate the stability of the shooting algorithm applied to the problem with control bounds (CP) studied in Section 8. Observe that previous Theorem 9.1 guarantees the weak optimality for the perturbed problem when the control constraints are absent. In case we have control constraints, this stability result is applied to the transformed problem (TP) (given by equations (94)-(98) of Section 8) yielding a similar stability property, but for which the nominal point and the perturbed ones are weak optimal for (TP). This means that they are optimal in the class of extremals having the same control structure, and switching times and singular arcs sufficiently close in L_∞ . An extremal satisfying optimality in this sense will be called *weak-structural optimal*, and a formal definition would be as follows:

Definition 9.5 (Weak-structural optimality). *A feasible solution \hat{w} for problem (CP) is called a weak-structural solution if its transformed extremal \hat{W} given by (99)-(101) is a weak solution of (TP).*

Theorem 9.6 (Sufficient condition for the extended weak minimum in the control constrained case). *Let \hat{w} be a feasible solution for (CP) satisfying Assumptions 8.1 and 8.2. Consider the transformed problem (TP) and the corresponding transformed solution \hat{W} given by (99)-(101). If \hat{w} satisfies (65) for (TP), then \hat{w} is an extended weak solution for (CP).*

Consider the family of perturbed problems given by:

$$\begin{aligned} \varphi_0^\mu(x_0, x_T) &\rightarrow \min, \\ \dot{x}_t &= \sum_{i=0}^m u_{i,t} f_i^\mu(x_t), \quad \text{for } t \in (0, T), \\ \eta^\mu(x_0, x_T) &= 0, \\ 0 &\leq u_t \leq 1, \quad \text{a.e on } (0, T). \end{aligned} \quad (\text{CP}_\mu)$$

The following stability result follows from the Theorem 9.1:

Theorem 9.7 (Stability in the control constrained case). *Assume that the shooting system generated by problem (CP) is square. Let \hat{w} be the solution of (CP) and $\{\hat{T}_k\}_{k=1}^N$ its switching times. Denote by \hat{W} its transformation via equation (101). Suppose that \hat{W} satisfies uniform positivity condition (65) for problem (TP). Then there exists a neighborhood $\mathcal{J} \subset \mathbb{R}$ of 0 such that for every parameter $\mu \in \mathcal{J}$ there exists a weak-structural optimal extremal w^μ of (CP^μ) with switching times $\{T_k^\mu\}_{k=1}^N$ satisfying the estimation*

$$\sum_{k=1}^N |T_k^\mu - \hat{T}_k| + \sum_{k=1}^N \sum_{i \in S_k} \|u_i^\mu - \hat{u}_i\|_{\infty, I_k^\mu \cap \hat{I}_k} + \|x^\mu - \hat{x}\|_\infty = \mathcal{O}(\mu), \quad (144)$$

where $I_k^\mu := (T_{k-1}^\mu, T_k^\mu)$. Furthermore, the trasformed perturbed solution W^μ verifies uniform positivity (126) and hence quadratic growth in the weak sense for problem (TP) holds, and the shooting algorithm for (CP_μ) is well-posed.

9.3 Additional analysis for the scalar control case

Consider a particular case where the control \hat{u} is scalar and consists of a concatenation of bang and singular arcs. This situation is encountered quite often in practice. The lemma below shows that the perturbed solution are Pontryagin extremals for (CP_μ) provided that the following assumption holds.

Assumption 9.8. (a) *The switching function H_u is never zero in the interior of a bang arc. Hence if $\hat{u} = 1$ on (t_1, t_2) then $H_u < 0$ on (t_1, t_2) , and if $\hat{u} = -1$ on (t_1, t_2) then $H_u > 0$ on (t_1, t_2) .*

(b) *If \hat{T}_k is a bang-to-bang switching time then $\dot{H}_u(\hat{T}_k) \neq 0$.*

The property (a) is called *strict complementarity for the control constraint*.

Lemma 9.9. *Suppose that \hat{u} is a scalar concatenation of bang and singular arcs satisfying Assumption 9.8. Let w^μ as in Theorem 9.7 above. Then w^μ is a Pontryagin extremal for (CP_μ) .*

Proof. We intend to prove that w^μ satisfies the minimum condition (10) given by the Pontryagin Maximum Principle. Observe that on the singular arcs, $H_u^\mu = 0$ since w^μ is the solution associated to a zero of the shooting function. It suffices then to study the stability of the sign of H_u^μ on the bang arcs around a switching time. First suppose that \hat{u} has a singular-to-bang switching at \hat{T}_k . Assume, without loss of generality, that $\hat{u} \equiv 1$ on $[\hat{T}_{k-1}, \hat{T}_k]$ and \hat{u} is singular on $[\hat{T}_k, \hat{T}_{k+1}]$. Let us write

$$\ddot{H}_u^\mu = a^\mu + u^\mu b^\mu, \quad (145)$$

where a^μ and $b^\mu := \frac{\partial}{\partial u} \ddot{H}_u^\mu$ are continous functions on $[0, T]$, and continuously differentiable with respect to μ since they depend on x^μ and p^μ . Assumption 8.3 yields $b^0 < 0$ on $[\hat{T}_k, \hat{T}_{k+1}]$, and therefore

$$b^\mu < 0, \quad \text{on } [T_k^\mu, T_{k+1}^\mu]. \quad (146)$$

Due to (145), the sign of \ddot{H}_u^μ around T_k^μ depends on $u^\mu(T_k^{\mu+}) - u^\mu(T_k^{\mu-})$. But this quantity is negative since u^μ passes from its upper bound to a singular arc. From the latter assertion and (146) follows

$$\ddot{H}_u^\mu(T_k^{\mu-}) < 0, \quad (147)$$

and thus H_u^μ is concave at the junction time T_k^μ . Since H_u^μ is null on $[T_k^\mu, T_{k+1}^\mu]$, its concavity implies that it has to be negative before entering this arc. Hence, w^μ respects the minimum condition on the interval $[\hat{T}_{k-1}, \hat{T}_k]$.

Consider now the case when \hat{u} has a bang-to-bang switching at \hat{T}_k . Let us begin by showing that $H_u^\mu(T_k^\mu) = 0$. Suppose on the contrary that $H_u^\mu(T_k^\mu) \neq 0$. Then $H^\mu(T_k^\mu+) - H^\mu(T_k^\mu-) \neq 0$, contradicting the continuity condition imposed on H in the shooting system. Hence $H_u^\mu(T_k^\mu) = 0$. On the other hand, since $\dot{H}_u(\hat{T}_k) \neq 0$ by Assumption 9.8, the value $\dot{H}_u^\mu(T_k^\mu)$ has the same sign for small μ . This implies that H_u^μ has the same sign before and after T_k^μ that H_u (before and after \hat{T}_k), respectively. The result follows. \square

Remark 9.10. *We end this analysis by mentioning that if the transformed solution \hat{W} satisfies the uniform positivity (65) for (TP), then \hat{w} verifies the sufficient condition established in Aronna et al. [2] and hence it is actually a Pontryagin minimum. This follows from the fact that in condition (65) we are allowed to perturb the switching times, and hence (65) is more restrictive than the condition in [2].*

10 Numerical simulations

Now we aim to check numerically the extended shooting method described above. More precisely, we want to compare the classical $n \times n$ shooting formulation to an extended formulation with the additional conditions on the Hamiltonian continuity. We test three problems with singular arcs: a fishing and a regulator problem and the well-known Goddard problem, which we have already studied in [18, 28]. For each problem, we perform a batch of shootings on a large grid around the solution. We then check the convergence and the solution found, as well as the singular values and condition number of the Jacobian matrix of the shooting function.

10.1 Test problems

10.1.1 Fishing problem

The first example we consider is a fishing problem described in [8]. The state $x(t) \in \mathbb{R}$ represents the fish population (halibut), the control $u(t) \in \mathbb{R}$ is the fishing activity, and the objective is to maximize the net revenue of fishing over a fixed time interval. The coefficient $(E - \frac{c}{x})$ takes into account the greater fishing cost for a low fish population.

$$\left\{ \begin{array}{l} \max \int_0^T (E - c/x(t)) u(t) U_{\max} dt, \\ \dot{x}(t) = rx(t) (1 - x(t)/k) - u(t) U_{\max}, \\ 0 \leq u(t) \leq 1, \quad \forall t \in [0, T], \\ x(0) = 70, \quad x(T) \text{ free}, \end{array} \right. \quad (\text{P}_1)$$

with $T = 10$, $E = 1$, $c = 17.5$, $r = 0.71$, $k = 80.5$ and $U_{\max} = 20$.

Remark 10.1. *The state and control were rescaled by a factor 10^6 compared to the original data for a better numerical behaviour.*

Remark 10.2. *Since we have an integral cost, we add a state variable to adapt (P_1) to the initial-final cost formulation. It is well-known that its corresponding costate variable is constantly equal to 1.*

The Hamiltonian for this problem is

$$H := (c/x - E)uU_{\max} + p[rx(1 - x/k) - uU_{\max}], \quad (148)$$

and hence the switching function

$$\Phi(t) = D_u H(t) = c/x(t) - E - p(t), \quad \forall t \in [0, T]. \quad (149)$$

The optimal control follows the bang-bang law

$$\begin{cases} u^*(t) = 0 & \text{if } \Phi(t) > 0, \\ u^*(t) = 1 & \text{if } \Phi(t) < 0. \end{cases} \quad (150)$$

Over a singular arc where $\Phi = 0$, we assume that the relation $\ddot{\Phi} = 0$ gives the expression of the singular control (*t is omitted for clarity*)

$$u_{\text{singular}}^* = \frac{k r}{2(c/x - p)U_{\max}} \left(\frac{c}{x} - \frac{c}{k} - p + \frac{2px}{k} - \frac{2px^2}{k^2} \right). \quad (151)$$

The solution obtained for (P_1) has the structure **bang-singular-bang**, as shown on Figure 1.

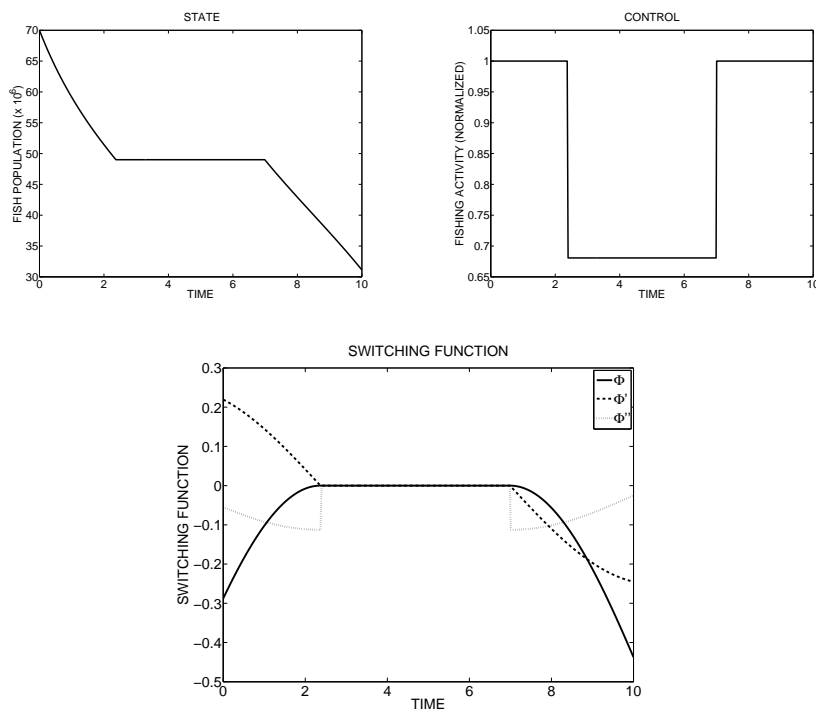


Figure 1: Fishing Problem

Shooting formulations. Assuming the control structure, the shooting unknowns are the initial costate and the limits of the singular arc,

$$\nu := (p(0), t_1, t_2) \in \mathbb{R}^3.$$

The classical shooting formulation uses the entry conditions on t_1

$$\mathcal{S}_1(\nu) := (p(T), \Phi(t_1), \dot{\Phi}(t_1)).$$

Solving $\mathcal{S}_1(\nu) = 0$ is a square nonlinear system, for which a quasi-Newton method can be used. Note that even if there is no explicit condition on t_2 in \mathcal{S} , the value of $p(T)$ does depend on t_2 via the control switch.

The extended shooting formulation adds two conditions corresponding to the continuity of the Hamiltonian at the junctions between bang and singular arcs. We denote $[H]_t := H(t+) - H(t-)$ the Hamiltonian jump, and define

$$\tilde{\mathcal{S}}_1(\nu) = (p(10), \Phi(t_1), \dot{\Phi}(t_1), [H]_{t_1}, [H]_{t_2}). \quad (152)$$

To solve $\tilde{\mathcal{S}}_1(\nu) = 0$ we use a nonlinear least-square algorithm (see paragraph 10.2 below for more details).

10.1.2 Regulator problem

The second example is the quadratic regulator problem described in [1]. We want to minimize the integral of the sum of the squares of the position and speed of a mobile over a fixed time interval, the control being the acceleration.

$$\left\{ \begin{array}{l} \min \frac{1}{2} \int_0^T (x_1^2(t) + x_2^2(t)) dt, \\ \dot{x}_1(t) = x_2(t), \\ \dot{x}_2(t) = u(t), \\ -1 \leq u(t) \leq 1, \quad \text{a.e. on } (0, T), \\ x(0) = (0, 1), \quad x(T) \text{ free}, \\ T = 5. \end{array} \right. \quad (\text{P}_2)$$

The corresponding Hamiltonian

$$H := \frac{1}{2}(x_1^2 + x_2^2) + p_1 x_2 + p_2 u, \quad (153)$$

and hence we have the switching function

$$\Phi(t) := D_u H(t) = p_2(t). \quad (154)$$

The bang-bang optimal control satisfies

$$u^*(t) = -\text{sign } p_2(t) \quad \text{if } \Phi(t) \neq 0. \quad (155)$$

The singular control is again obtained from $\ddot{\Phi} = 0$ and verifies

$$u_{\text{singular}}^*(t) = x_1(t). \quad (156)$$

The solution for this problem has the structure **bang-singular**, as shown on Figure 2.

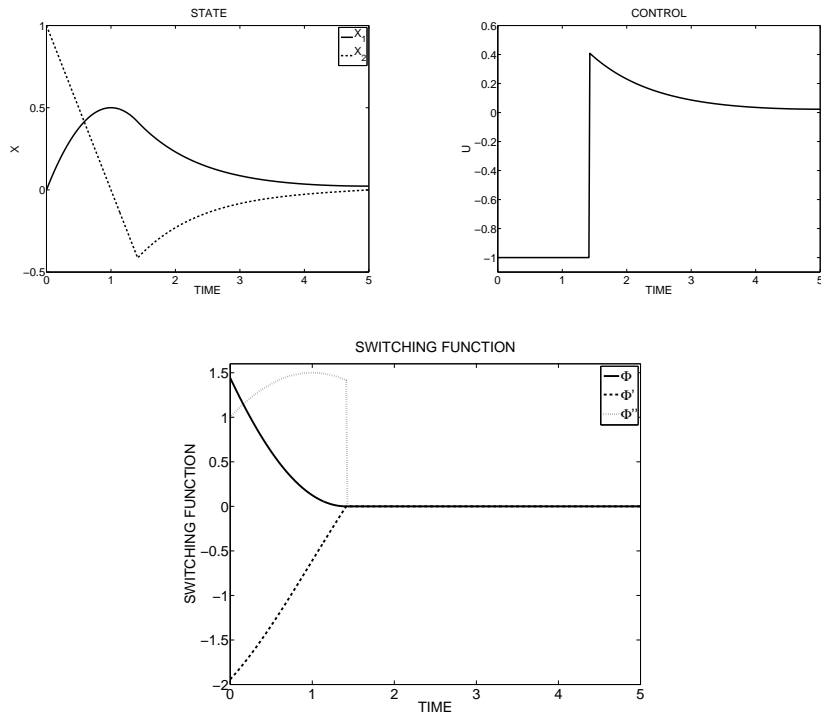


Figure 2: Regulator Problem

Shooting formulations. Assuming the control structure, the shooting unknowns are

$$\nu := (p_1(0), p_2(0), t_1) \in \mathbb{R}^3. \quad (157)$$

For the classical shooting formulation, in order to have a square system, we have to combine the two entry conditions on Φ and $\dot{\Phi}$, since we only have one additional unknown which is the entry time t_1 . Thus we define

$$\mathcal{S}_2(\nu) := (p_1(T), p_2(T), \Phi(t_1)^2 + \dot{\Phi}(t_1)^2). \quad (158)$$

The extended formulation does not require such a trick, we simply have

$$\tilde{\mathcal{S}}_2(\nu) := (p_1(T), p_2(T), \Phi(t_1), \dot{\Phi}(t_1), [H]_{t_1}). \quad (159)$$

10.1.3 Goddard problem

The third example is the well-known Goddard problem, studied for instance in [33]. This problem models the ascent of a rocket through the atmosphere, and we restrict here ourselves to vertical (monodimensional) trajectories. The state variables are the altitude, speed and mass of the rocket during the flight, for a total dimension of 3. The rocket is subject to gravity, thrust and drag forces. The final time is free, and the objective is to reach a certain altitude with a

minimal fuel consumption, i.e., a maximal final mass.

$$\left\{ \begin{array}{l} \max m(T), \\ \dot{r} = v, \\ \dot{v} = -1/r^2 + 1/m(T_{\max}u - D(r, v)) \\ \dot{m} = -bT_{\max}u, \\ 0 \leq u(t) \leq 1, \quad \text{a.e. on } (0, 1), \\ r(0) = 1, v(0) = 0, m(0) = 1, \\ r(T) = 1.01, \\ T \text{ free,} \end{array} \right. \quad (P_3)$$

with the parameters $b = 7$, $T_{\max} = 3.5$ and the drag given by $D(r, v) := 310v^2e^{-500(r-1)}$. The Hamiltonian function here is

$$H := p_r v + p_v (-1/r^2 + 1/m(T_{\max}u - D(r, v))) - p_m b T_{\max}u, \quad (160)$$

where p_r , p_v and p_m are the costate variables associated to r , v and m , respectively. The switching function is

$$\Phi := D_u H = T_{\max}((1 - p_m)b + p_v/m). \quad (161)$$

Hence, the bang-bang optimal control is given by

$$\begin{cases} u^*(t) = 0 & \text{if } \Phi(t) > 0, \\ u^*(t) = 1 & \text{if } \Phi(t) < 0, \end{cases} \quad (162)$$

and the singular control can be obtained by formally solving $\ddot{\Phi} = 0$. The expression of u_{singular}^* , however, is quite complicated and is not recalled here. The solution for this problem has the well-known typical structure **1-singular-0**, as shown on Figures 3 and 4.

Shooting formulations. Once again fixing the control structure, the shooting unknowns are

$$\nu = (p_1(0), p_2(0), p_3(0), t_1, t_2, T) \in \mathbb{R}^6. \quad (163)$$

Here is the classical shooting formulation with the entry conditions on t_1

$$\mathcal{S}_3(\nu) := (x_1(T) - 1.01, p_2(T), p_3(T) + 1, \Phi(t_1), \dot{\Phi}(t_1), H(T)), \quad (164)$$

while the extended formulation is

$$\tilde{\mathcal{S}}_3(\nu) := (x_1(T) - 1.01, p_2(T), p_3(T) + 1, \Phi(t_1), \dot{\Phi}(t_1), H(T), [H]_{t_1}, [H]_{t_2}). \quad (165)$$

10.2 Results

All tests were run on a 12-core platform, with the parallelized (OPENMP) version of the SHOOT ([29]) package. The ODE solver is a fixed step 4th. order Runge Kutta method with 500 steps. The classical shooting is solved with a basic Newton method, and the extended shooting with a basic Gauss-Newton method. Both algorithms use a fixed steplength of 1 and a maximum of 1000 iterations. In addition to the singular/bang structure, the value of the control on the bang arcs is also fixed according to the expected solution.

The values for the initial costates are taken in $[-10, 10]$, and the values for the entry/exit times in $[0, T]$ for (P_1) and (P_2) . For (P_3) , the entry, exit and

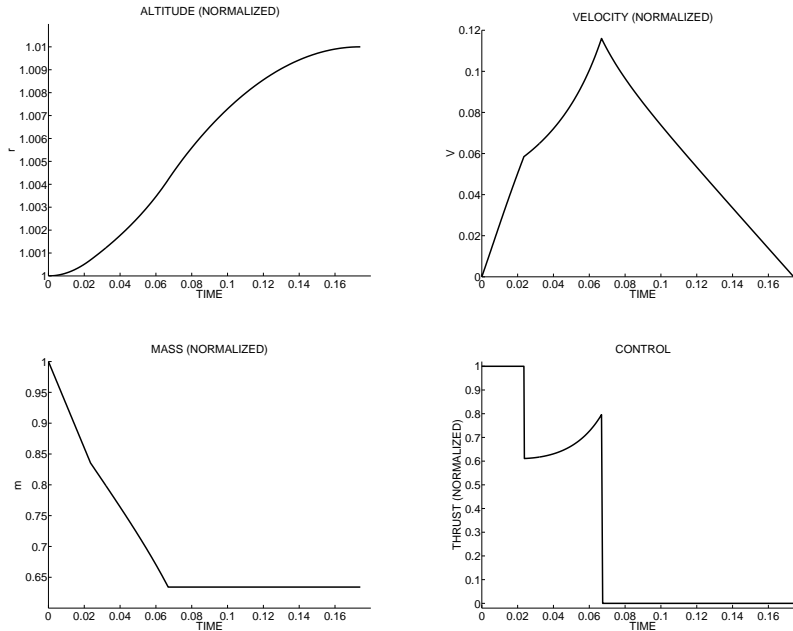


Figure 3: Goddard Problem

final times are taken in $[0, 0.2]$. The number of gridpoints is set around to 10 000 for the three problems. These grids for the starting points are quite large and rough, which explains the low success rate for (P_1) and (P_3) . However, the solution was found for all three problems.

For each problem, the results are summarized in 3 tables. The first table indicates the total CPU time for all shootings over the grid, the success rate of convergence to the solution, the norm of the shooting function at the solution, and the objective value. The second table recalls the solution found by both formulations: initial costate and junction times, as well as final time for (P_3) . The third table gives the singular values for the Jacobian matrix at the solution, as well as its condition number $\kappa := \sigma_1/\sigma_n$.

We observe that for all three problems (P_1) , (P_2) and (P_3) , both formulations converge to the same solution, ν^* and the objective being identical to more than 6 digits. The success rate over the grid, total CPU time and norm of the shooting function at the solution are close for both formulations. Concerning the singular values and condition number of the Jacobian matrix, we note that for (P_2) the extended formulation has the smallest singular value going from 10^{-8} to 1, thus improving the condition number by a factor 10^8 . This may be caused by the combination of the two entry conditions into a single one that we had to use in the classical formulation for this problem: as the singular arc lasts until t_f , there is only one additional unknown: the entry time.

Overall, these results validate the extended shooting formulation, which perform at least as well as the classical formulation and has a theoretical foundation.

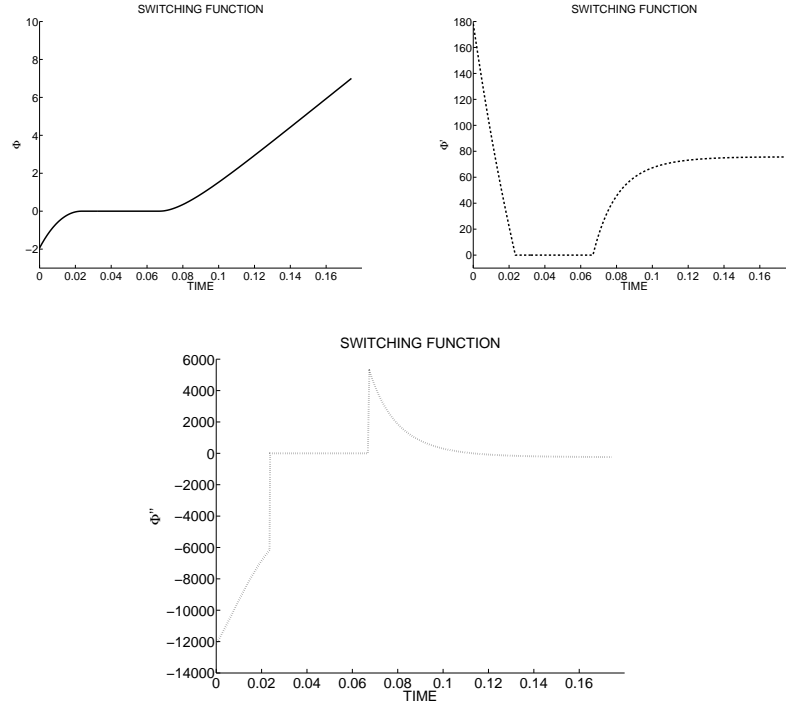


Figure 4: Goddard Problem

Remark 10.3. Several additional tests runs were made using the *HYBRD* ([17]) and *NL2SNO* ([10]) solvers for the classical and extended shootings. The results were similar, apart from a higher succes rate for the *HYBRD* solver compared to *NL2SNO*.

Remark 10.4. We also tested both formulations using the sign of the switching function to determine the control value over the bang arcs, instead of forcing the value. However, this causes a numerical instability at the exit of a singular arc, where the switching function is supposed to be 0 but whose sign determines the control at the beginning of the following bang arc. This instability leads to much more erratic results for both shooting formulations, but with the same general tendencies.

Problem 1:

Shooting grid: $[-10, 10] \times [0, T]^2$, 21^3 gridpoints, 9261 shootings.

Shooting	CPU	Success	Convergence	Objective
Classical	74 s	21.28 %	1.43E-16	-106.9059979
Extended	86 s	22.52 %	6.51E-16	-106.9059979

Table 1.1: (P_1) CPU times, success rate, convergence and objective

Shooting	$p(0)$	t_1	t_2
Classical	-0.462254744307241	2.37041478456004	6.98877992494185
Extended	-0.462254744307242	2.37041478456004	6.98877992494185

Table 1.2: (P_1) solution ν^* found

Shooting	σ_1	σ_2	σ_3	κ
Classical	3.61	0.43	5.63E-02	64.12
Extended	27.2	1.71	3.53E-01	77.05

Table 1.3: (P_1) singular values and condition number for the Jacobian**Problem 2**

Shooting grid: $[-10, 10]^2 \times [0, T]$, 21^3 gridpoints, 9261 shootings.

Shooting	CPU	Success	Convergence	Objective
Classical	468 s	94.14 %	1.17E-16	0.37699193037
Extended	419 s	99.36 %	1.22E-13	0.37699193037

Table 2.1: (P_2) CPU times, success rate, convergence and objective

Shooting	$p_1(0)$	$p_2(0)$	t_1
Classical	0.942173346483640	1.44191017584598	1.41376408762863
Extended	0.942173346476773	1.44191017581021	1.41376408762893

Table 2.2: (P_2) solution ν^* found

Shooting	σ_1	σ_2	σ_3	κ
Classical	24.66	5.19	1.96E-08	1.26E+09
Extended	24.70	5.97	1.13	21.86

Table 2.3: (P_2) singular values and condition number for the Jacobian**Problem 3**

Shooting grid: $[-10, 10]^3 \times [0, 0.2]^3$, $4^3 \times 5^3$ gridpoints, 8000 shootings.

Shooting	CPU	Success	Convergence	Objective
Classical	42 s	0.82 %	5.27E-13	-0.634130666
Extended	52 s	0.85 %	1.29E-10	-0.634130666

Table 3.1: (P_3) CPU times, success rate, convergence and objective

Shooting	$p_r(0)$	$p_v(0)$	$p_m(0)$
Classical	-50.9280055899288	-1.94115676279896	-0.693270270795148
Extended	-50.9280055901093	-1.94115676280611	-0.693270270787320
	t_1	t_2	t_f
Classical	0.02350968417421373	0.06684546924474312	0.174129456729642
Extended	0.02350968417420884	0.06684546924565564	0.174129456733106

Table 3.2: (P_3) solution ν^* found

Shooting	σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	κ
Classical	6182	9.44	8.13	2.46	0.86	1.09E-03	5.67E+06
Extended	6189	12.30	8.23	2.49	0.86	1.09E-03	5.67E+06

Table 3.3: (P_3) singular values and condition number for the Jacobian

11 Conclusion

Theorems 5.6 and 8.8 provide for the first time a theoretical support for a numerical method for singular problems. The shooting functions presented both in (23) and (124) are not the ones usually implemented in numerical methods as we have already pointed out in previous section. They come from systems having more equations than unknowns in the general case, while in practice square systems are usually used. Anyway, we are not able to prove the injectivity of \mathcal{S} when we remove some equations, i.e., we are not able to determine which equations are redundant, and we suspect that it can vary for different problems.

The proposed algorithm was tested in three problems, where we compared its performance with the classical shooting method for square systems. The percentages of convergence are similar in both approaches, the singular values and condition number of the Jacobian matrix of the shooting function coincide in two problems, and are better for our formulation in one of the problems. Summarizing, we can observe that the proposed method works as well as the one currently used in practice and has a theoretical foundation.

In the case bang-singular-bang, as in the fishing and Goddard's problems, our formulation coincides with the algorithm proposed by Maurer [30].

In case we have a square system, given that the sufficient condition for the non-singularity of the Jacobian of the shooting function coincides with a sufficient condition for optimality we could guarantee for the first time the stability of the optimal local solution under small perturbations of the data.

It would be interesting to extend this result of well-posedness to a more general framework having, for instance, nonlinear mixed state-control path constraints.

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