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# Approximation of chattering arcs in optimal control problems governed by mono-input affine control systems

Térence Bayen<sup>\*</sup>, F. Mairet<sup>†</sup>

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#### Abstract

In this paper, we consider a general Mayer optimal control problem governed by a mono-input affine control system whose optimal solution involves a second-order singular arc (leading to chattering). The objective of the paper is to present a numerical scheme to approach the chattering control by controls with a simpler structure (concatenation of bang-bang controls with a finite number of switching times and first-order singular arcs). Doing so, we consider a sequence of vector fields converging to the drift such that the associated optimal control problems involve only first-order singular arcs (and thus, optimal controls necessarily have a finite number of bang arcs). Up to a subsequence, we prove convergence of the sequence of extremals to an extremal of the original optimal control problem as well as convergence of the value functions. Next, we consider several examples of problems involving chattering. For each of them, we give an explicit family of approximated optimal control problems whose solutions involve bang arcs and first-order singular arcs. This allows us to approximate numerically solutions (with chattering) to these original optimal control problems.

Keywords : optimal control, singular arcs, chattering, numerical methods.

## 1 Introduction

In numerous optimal control problems arising in various areas such as aerospace, biology, mechanics, the optimal solution involves what is called *Fuller's phenomenon*. In that case, we also say that *chattering* occurs. This property means that the optimal control possesses an infinite number of extremal bang arcs over a finite time interval. This particularly interesting behavior of optimal controls was originally discovered by A.T. Fuller in the seminal works [10, 11, 12]. Since then, many properties related to chattering were studied by several authors (see, *e.g.*, [20] and the monograph [27] giving a large panel on the chattering phenomenon).

Fuller's phenomenon arises whenever an optimal control problem presents a second order singular arc. Recall that in geometric optimal control theory, a singular singular arc is a time interval on which the optimal control takes values within the interior of the admissible control set. The occurrence of such arcs is of utmost importance to compute an optimal solution since it completely determines the optimal synthesis. This situation is encountered typically when computing minimum time syntheses in the two-dimensional setting in presence of a turnpike singular arc (see [4] or [2]). In the setting of Mayer optimal control problems governed by an affine control system, the application of the Pontryagin maximum Principle (in short, PMP) shows that several cases may occur (see, e.g., [7]). First, geometric control theory predicts that the control input is present explicitly in the expression defining the derivative of order  $2n, n \geq 1$ , of the switching function. So, if the control input is present in the second-order derivative of the switching function (allowing to compute the singular control as a function of the state and co-state), then, we say that a singular arc of first order occurs. But, it may happen that the control is present explicitly only in the fourth-order derivative of the switching function (and not in the second-order derivative) leading that way to a second-order singular arc and to chattering, see, e.g., [27, 21]. More generally, it is possible to encounter optimal control problems involving singular arcs of order greater than three. But, we shall restrict our attention here to the case of first and second order singular arcs that are the most common ones in the application models.

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A striking point related to second order singular arcs is that they arise in simple examples from mathematical modeling such as in aerospace [28, 29], in biomedicine [15, 14, 22], in biology [16, 17], or in physics [19]. The simplest problem involving chattering is known as Fuller's problem for which the underlying system is the two-dimensional double integrator associated with a quadratic cost. It is worth noticing that chattering renders the analysis of optimal solutions more delicate than for instance in the case of a first-order singular arc for which the optimal synthesis involves in general a low number of switching times. In particular, the occurrence of chattering raises the question of implementation of an optimal solution from a practical viewpoint. The question is how to bypass non-implementable solutions and how synthesizing an adequate sub-optimal control (typically based on a finite number of bang-bang arcs). This question was studied by several authors for instance in [6] by modifying the objective function via bounded variation controls.

In the present paper, we consider another approach to tackle chattering based on a perturbation technique. More precisely, we consider a general optimal control problem governed by a mono-input affine control system whose optimal solution involves a second-order singular arc. We suppose that there is a sequence of dynamics converging to the original one such that the associated optimal solution involves only first-order singular arcs. This sequence is constructed by approximating the drift term. From a practical viewpoint, we thus approach the original optimal control by a perturbed one for which the optimal solution does not involve chattering. We first prove that, up to a sub-sequence, an extremal of the perturbed optimal control problems converges to an extremal to the original optimal control problem. As well, we prove the convergence of the value function associated to the perturbed optimal control problem to the value function associated with the original optimal control problem. Convergence of optimal controls (up to a sub-sequence) is also guaranteed on time intervals for which the limit trajectory is non-singular. Interestingly, the approximated optimal control is a concatenation of a finite number of bang and singular arcs. Next, we show how to construct such approximating sequence on three examples with chattering : a variation on Fuller's problem, a resource-allocation model [13], and a quantum control system [19].

The paper is organized as follows. In Section 2, we introduce our methodology and we prove convergence results between the sequence of approximated optimal control problems and the original optimal control problem. Next, in Section 3, we address three examples for which we provide an explicit sequence of approximated optimal control problems. For each of them, we verify that the limit problem possesses chattering whereas perturbed optimal control problems involve only first-order singular arcs. In addition, for each example, we provide numerical solutions (with an increasing number of arcs as the sequence approaches the original dynamics) to the approximated optimal control problems via a direct method [23].

# 2 Approximation and convergence result

## 2.1 Second order singular arcs

Hereafter, we denote by  $A^{\top}$  the transpose of a matrix A and the inner product in the Euclidean space is written  $a \cdot b$  where a, b are two vectors. Let  $n \in \mathbb{N}^*$  and consider two vector fields  $f, g : \mathbb{R}^n \to \mathbb{R}^n$  of class  $C^{\infty}$ , a terminal pay-off  $\psi : \mathbb{R}^n \to \mathbb{R}$  of class  $C^1$ , and let C be a non-empty closed convex subset of  $\mathbb{R}^n$ . Given T > 0and  $x_0 \in \mathbb{R}^n$ , we consider the Mayer optimal control problem

$$\inf_{u \in \mathcal{U}} \psi(x(T)) \quad \text{s.t.} \begin{cases} \dot{x}(t) &= f(x(t)) + u(t)g(x(t)) \quad \text{a.e. } t \in [0,T], \\ x(0) &= x_0, \\ x(T) &\in C, \end{cases}$$
(OCP)

where  $\mathcal{U}$  denotes the set of admissible controls  $u: [0, T] \to [-1, 1]$  that are measurable. The aim of this paper is to provide alternative strategies in order to study (OCP) whenever f and g satisfy the condition:

$$[g, [f, g]] = 0 \quad \text{over } \mathbb{R}^n, \tag{2.1}$$

or whenever the covector is orthogonal to [g, [f, g]] along a singular arc, where  $[f, g](x) := D_x g(x) f(x) - D_x f(x)g(x)$  denotes the Lie bracket of f and g and where  $D_x f(x)$ ,  $D_x g(x)$  stand respectively for the Jacobian matrix of f and g. Under one of these two conditions, we know that optimal controls may involve an infinite number of switching times over [0, T]. This phenomenon renders the analysis of optimal trajectories quite involved (*e.g.*, the determination of the switching locus in this context). Thus, from a numerical point of view, it is desirable to deal with controls having a finite number of switching times.

First, we would like to remind why condition (2.1) implies the so-called Fuller's phenomenon (or chattering). From Pontryagin's Principle [18, 24], if u is an optimal control and x denotes the associated solution of the system defined over [0,T], there exist  $p^0 \leq 0$  and an absolutely continuous function  $p : [0,T] \to \mathbb{R}^n$  (the covector) satisfying the adjoint equation

$$\dot{p}(t) = -D_x f(x(t))^\top p(t) - u(t) D_x g(x(t))^\top p(t)$$
 a.e.  $t \in [0, T],$  (2.2)

together with the transversality condition

$$p(T) + p^0 \nabla \psi(x(T)) \in -N_C(x(T)), \qquad (2.3)$$

where  $N_C(x)$  denotes the (convex) normal cone to the set C at some point  $x \in C$ . The pair  $(p^0, p(\cdot))$  also fulfills the non-triviality condition  $(p^0, p(\cdot)) \neq 0$ . Finally, the Hamiltonian maximization condition gives us the following control law:

$$u(t) = \text{sign}(\phi(t))$$
 a.e.  $t \in [0, T]$  s.t.  $\phi(t) \neq 0$ , (2.4)

where  $\phi(t) := p(t) \cdot g(x(t))$  is the switching function. On a sub-interval  $[t_1, t_2] \subset [0, T]$  on which  $\phi$  vanishes, a different analysis should be carried out in order to find the expression of an optimal control (in particular (2.4) is useless). If this situation occurs, then, we say that the extremal<sup>1</sup> (x, p, u) is *singular* over  $[t_1, t_2]$ (equivalently, we say that the trajectory has a singular arc over  $[t_1, t_2]$ ). The study of singular arcs relies on the expressions defining the derivatives of  $\phi$  w.r.t. the time. A simple computation shows that one has

$$\phi(t) = p(t) \cdot [f, g](x(t)), \quad t \in [0, T],$$

and that

$$\ddot{\phi}(t) = p(t) \cdot [f, [f, g]](x(t)) + u(t)p(t) \cdot [g, [f, g]](x(t)) \quad \text{a.e. } t \in [0, T].$$
(2.5)

Thus, under (2.1), if a singular arc occurs, the (corresponding) singular control u cannot be expressed thanks to (2.5), but further derivations of  $\ddot{\phi}$  are needed to compute the singular control (at least two according to the geometric control theory). This leads to the singular arcs of order at least two. In this direction, let us remind the following result about the occurrence of the chattering phenomenon for second-order singular arcs (see [21]).

**Proposition 2.1.** Suppose that (2.1) is fulfilled. Consider a normal extremal (x, p, u) containing a singular arc over  $[t_1, t_2]$ . Suppose that one has

$$\forall t \in [t_1, t_2], \ p(t) \cdot [g, [f, [f, g]]] | (x(t)) > 0, \tag{2.6}$$

and that the corresponding singular control is admissible over  $[t_1, t_2]$ . Then, the singular arc is of second order and it cannot be concatenated with a bang arc.

This means that the only possibility for an optimal control to connect the trajectory to the singular arc is an infinite sequence of bang arcs since the proposition excludes the concatenation of the singular arc to the optimal trajectory by a finite number of bang arcs. Also, singular controls may exceed the largest admissible value leading to saturation [1], that is why, the singular control is supposed to be admissible in Proposition 2.1. In addition to this proposition, let us also recall Legendre-Clebsch's condition [21] in the above context (with a single input). If a singular arc of order<sup>2</sup>  $q \in \mathbb{N}^*$  is optimal over some time interval  $[t_1, t_2]$ , then it must satisfy the condition

$$-\frac{\partial}{\partial u}\frac{d^{2q}}{dt^{2q}}\phi \le 0.$$

If this inequality is strict, we then speak of the strict Legendre-Clebsch condition. Typically, if q = 1, then,  $\phi$  must satisfy  $\ddot{\phi}_{|_{u}} > 0$  along a singular arc whereas if q = 2, then, it must satisfy  $\ddot{\phi}_{|_{u}} = 0$  and  $\ddot{\phi}_{|_{u}} < 0$ .

<sup>&</sup>lt;sup>1</sup>An extremal is a triple (x, p, u) satisfying the state-adjoint system, the transversality condition, and the Hamiltonian maximization condition.

<sup>&</sup>lt;sup>2</sup>We mean that along a singular arc, the input is present explicitly in the expression of  $\phi^{(2q)}$  and not in  $\phi^{(2r)}$ , r = 1, ..., q - 1.

## 2.2 Approximation of the optimal control problem

In order to avoid Fuller's phenomenon, we propose the following approach. We suppose that there is a sequence  $f_k : \mathbb{R}^n \to \mathbb{R}^n$  (of class  $C^{\infty}$  for each  $k \in \mathbb{N}$ ) such that

$$\|f_k - f\|_{L^\infty} \to 0, \tag{2.7}$$

together with

$$\|D_x f_k - D_x f\|_{L^\infty} \to 0, \tag{2.8}$$

as  $k \to +\infty$  (where  $L^{\infty} := L^{\infty}(\mathbb{R}^n)$  is the set of bounded functions) and such that

$$[g, [f_k, g]] \neq 0 \quad \text{over } \mathbb{R}^n, \tag{2.9}$$

for every  $k \in \mathbb{N}$ . This hypothesis will allow us to prevent chattering (see the discussion in Section 2.4). Consider now the approximated Mayer optimal control problem:

$$\inf_{u \in \mathcal{U}} \psi(x(T)) \quad \text{s.t.} \begin{cases} \dot{x}(t) &= f_k(x(t)) + u(t)g(x(t)) \quad \text{a.e. } t \in [0, T], \\ x(0) &= x_0, \\ x(T) &\in C, \end{cases}$$
(OCP<sub>k</sub>)

and let us introduce additional hypotheses in order to ensure existence of solutions to (OCP) and (OCP<sub>k</sub>). Hereafter  $|\cdot|$  denotes the Euclidean norm in  $\mathbb{R}^n$ .

**Assumption 2.1.** We suppose that for every  $k \in \mathbb{N}$ , the target set C is reachable from  $x_0$  for the controlled dynamics

$$\dot{x}(t) = f_k(x(t)) + u(t)g(x(t))$$
 a.e.  $t \in [0, T],$  (2.10)

where  $u \in \mathcal{U}$ . Similarly, we assume that C is also reachable from  $x_0$  for the controlled dynamics

$$\dot{x}(t) = f(x(t)) + u(t)g(x(t))$$
 a.e.  $t \in [0, T],$  (2.11)

where  $u \in \mathcal{U}$ . In addition, we suppose that there is  $c \geq 0$  such that

$$\forall k \in \mathbb{N}, \ |f_k(x)| \le c(|x|+1) \ ; \ |f(x)| \le c(|x|+1) \ ; \ |g(x)| \le c(|x|+1) \quad \text{for all } x \in \mathbb{R}^n.$$
(2.12)

Note that for simplicity, we supposed that the sequence  $(f_k)$  satisfies a linear growth condition, but this hypothesis could be removed in view of (2.7).

**Lemma 2.1.** If Assumption 2.1 is satisfied, then for every  $k \in \mathbb{N}$ , (OCP<sub>k</sub>) has a solution as well as (OCP).

*Proof.* Since the velocity sets associated to (2.10) and (2.11) are convex w.r.t. u, we can apply Filipov's existence Theorem (see [8]), whence the result.

#### 2.3 Convergence results

For every  $k \in \mathbb{N}$ , let  $u_k$  be an optimal solution of (OCP<sub>k</sub>). According to the PMP, there exist  $p_k^0 \leq 0$  and an absolutely continuous function  $p_k : [0,T] \to \mathbb{R}^n$  such that  $(p_k^0, p_k(\cdot)) \neq 0$  and such that

$$\dot{p}_k(t) = -D_x f_k(x_k(t))^\top p_k(t) - u_k(t) D_x g(x_k(t))^\top p_k(t) \quad \text{a.e. } t \in [0, T],$$
(2.13)

together with the transversality condition

$$p_k(T) + p_k^0 \nabla \psi(x_k(T)) \in -N_C(x_k(T)).$$
 (2.14)

In addition, the Hamiltonian maximization condition implies that

$$u_k(t) = \operatorname{sign}(\phi_k(t))$$
 a.e.  $t \in [0, T]$  s.t.  $\phi_k(t) \neq 0$ , (2.15)

where  $\phi_k(t) := p_k(t) \cdot g(x_k(t))$ . Finally, since the problem is autonomous the Hamiltonian of the problem is constant almost everywhere, that is, for all  $k \in \mathbb{N}$ , there is  $H_k \in \mathbb{R}$  such that

$$H_k := p_k(t) \cdot f_k(x_k(t)) + u_k(t)p_k(t) \cdot g(x_k(t))$$
 a.e.  $t \in [0, T]$ .

The transversality condition (2.14) implies that for every  $k \in \mathbb{N}$ , there exists  $\xi_k \in N_C(x_k(T))$  such that

$$p_k(T) + p_k^0 \nabla \psi(x_k(T)) = -\xi_k,$$

so, the scalar  $r_k := \sqrt{(p_k^0)^2 + |\xi_k|^2}$  is with positive value for all  $k \in \mathbb{N}$  since the pair  $(p_k^0, p_k(\cdot))$  is non-trivial. Hence, we can set

$$q_k := p_k / r_k. \tag{2.16}$$

Hereafter, we say that a sequence  $(x_k)$  of absolutely continuous functions over [0, T] strongly-weakly converges to a function  $x^* : [0, T] \to \mathbb{R}^n$  if and only if  $||x_k - x^*||_{L^{\infty}([0,T]; \mathbb{R}^n)} \to 0$  and  $\dot{x}_k \rightharpoonup \dot{x}^*$  (weak convergence in  $L^2([0,T]; \mathbb{R}^n)$ ).

**Proposition 2.2.** Suppose that Assumption 2.1 is satisfied. For every  $k \in \mathbb{N}$ , denote by  $u_k$  an optimal solution of  $(OCP_k)$  and let  $q_k$  be defined by (2.13)-(2.14), and (2.16). Then, there exists an extremal  $(x^*, p, u^*)$  associated with (OCP) such that, up to a sub-sequence,  $(x_k, q_k)$  strongly-weakly converges to  $(x^*, p)$  over [0, T]. In addition, one has the pointwise convergence  $u_k(t) \to u^*(t)$  on every time interval  $[t_1, t_2]$  such that  $\phi(t) \neq 0$  where  $\phi(t) := p(t) \cdot g(x^*(t)), t \in [0, T]$ . In addition,  $u^*$  is an optimal solution to (OCP).

*Proof.* From the linear growth assumption on the sequence of dynamics  $(f_k)$  and f (Assumption 2.1), we easily obtain that the sequence  $(x_k)$  is uniformly bounded over [0, T] since the set of admissible controls is bounded. So, the sequence  $(x_k(T))$  is also bounded, hence, up to a subsequence, we may assume that it converges to some value  $w \in \mathbb{R}^n$ . Now, let us set  $\alpha_k := p_k^0/r_k$  and  $\beta_k := -\xi_k/r_k$  so that the transversality condition reads as follows:

$$q_k(T) + \alpha_k \nabla \psi(x_k(T)) = \beta_k$$

By compacteness of the unit ball in  $\mathbb{R}^{1+n}$ , we may assume (extracting a sub-sequence if necessary) that the sequence  $(\alpha_k, \beta_k)_k$  converges to a limit  $(\alpha, \beta) \in \mathbb{R}^{1+n}$  which is non-zero and such that  $\alpha \leq 0$ . By closedness property of the normal cone, one also obtains that  $-\beta \in N_C(w)$ . Next, observe that the Hamiltonian of the problem and that the adjoint equation are linear w.r.t. the covector, so the triple  $(x_k, q_k, u_k)$  satisfies:

$$\tilde{H}_k := \frac{H_k}{r_k} = q_k(t) \cdot f_k(x_k(t)) + u_k(t)q_k(t) \cdot g(x_k(t)) \quad \text{a.e. } t \in [0,T],$$
(2.17)

together with the state-adjoint system

$$\begin{cases} \dot{x}_k(t) = f(x_k(t)) + u_k(t)g(x_k(t)) + \hat{\eta}_k(t), \\ \dot{q}_k(t) = -D_x f(x_k(t))^\top q_k(t) - u_k(t)D_x g(x_k(t))^\top q_k(t) + \tilde{\eta}_k(t), \end{cases}$$
(2.18)

where for a.e.  $t \in [0, T]$ ,  $\hat{\eta}_k(t)$  and  $\tilde{\eta}_k(t)$  are defined as:

$$\hat{\eta}_k(t) := f_k(x_k(t)) - f(x_k(t)) \quad ; \quad \tilde{\eta}_k(t) := D_x f(x_k(t))^\top q_k(t) - D_x f_k(x_k(t))^\top q_k(t).$$

Setting  $z_k := (x_k, q_k)$  and using that  $(x_k)$  is uniformly bounded over [0, T], we obtain that there exists  $c' \ge 0$  such that for every  $k \in \mathbb{N}$  one has

$$|z_k(t)| \le c'(|z_k(t)| + 1)$$
 a.e.  $t \in [0, T],$  (2.19)

where  $|\cdot|$  denotes the Euclidean norm in  $\mathbb{R}^{2n}$ . From the preceding inequality and the fact that  $(x_k(T), q_k(T))$  converges, we obtain after application of Gronwall's Lemma that  $(x_k(\cdot), q_k(\cdot))$  is uniformly bounded over [0, T]. Now the multi-function

$$F(x,q) := \{ (f(x) + ug(x), -D_x f(x)^\top q - uD_x g_k(x)^\top q) ; u \in [-1,1] \},\$$

is with compact convex values for every  $(x,q) \in \mathbb{R}^{2n}$ . Remind that  $z_k(T)$  converges and note also (using the uniform boundedness of  $(x_k, q_k)$  in  $L^{\infty}([0,T]; \mathbb{R}^n)$ ) that the sequences  $\hat{\eta}_k(\cdot)$  and  $\tilde{\eta}_k(\cdot)$  uniformly converge to zero. Hence, we can apply [9, Theorem 1.11] which shows the existence of an absolutely continuous pair  $(x^*, p)$  as well as a control function  $u^* \in \mathcal{U}$  such that

$$\begin{cases} \dot{x}^{\star}(t) = f(x^{\star}(t)) + u^{\star}(t)g(x^{\star}(t)), \\ \dot{p}(t) = -D_{x}f(x^{\star}(t))^{\top}p(t) - u^{\star}(t)D_{x}g(x^{\star}(t))^{\top}p(t), \end{cases}$$
(2.20)

for a.e.  $t \in [0, T]$ . In addition,  $(x_k, q_k)$  strongly-weakly converges to  $(x^*, p)$  over [0, T]. Also, by passing to the limit as  $k \to +\infty$ , we obtain that  $x^*(0) = x_0$  and that  $p(T) + \alpha \nabla \psi(x^*(T)) = \beta \in -N_C(x^*(T))$  (using the closedness property of the normal cone) where  $(\alpha, \beta)$  is non-zero and  $\alpha \leq 0$ . This proves the first property of Proposition 2.2.

Let us now address convergence of the sequence of controls  $(u_k)$  to  $u^*$ . Suppose that there is  $t_0 \in [0, T]$ such that  $\phi(t_0) > 0$ . By uniform convergence of  $\phi_k$  to  $\phi$ , there exist  $k_0 \in \mathbb{N}$ ,  $\varepsilon > 0$ , and  $\kappa > 0$  such that for every  $k \ge k_0$  and every  $t \in [t_0 - \varepsilon, t_0]$ , one has  $\phi_k(t) \ge \kappa$ . Thus, by the Hamiltonian maximization condition, we obtain that  $u_k(t) = +1$  for every  $t \in [t_0 - \varepsilon, t_0]$  and every  $k \ge k_0$ . Hence, for all  $\eta \in (0, \varepsilon)$  and for all  $k \ge k_0$ , one has

$$\frac{1}{\eta} \int_{t_0-\eta}^{t_0} \dot{x}_k(t) \, \mathrm{d}t = \frac{1}{\eta} \int_{t_0-\eta}^{t_0} [f_k(x_k(t)) + g(x_k(t))] \, \mathrm{d}t.$$

Thus, if we let  $k \to +\infty$  (utilizing uniform convergence of the sequences  $(f_k)$  and  $(x_k)$  and also weak convergence of  $(\dot{x}_k)$ ) and next  $\eta \downarrow 0$ , one obtains using that almost every  $t_0 \in [0, T]$  is a Lebesgue point of  $u^*$  (since  $u^*$  is bounded):

$$\dot{x}^{\star}(t_0) = f(x^{\star}(t_0)) + g(x^{\star}(t_0)).$$

It follows that  $u^*(t_0) = +1 = \operatorname{sign}(\phi(x^*(t_0)))$ . By repeating this argumentation in a neighborhood of every point  $t_0 \in [0, T]$  such that  $\phi(x^*(t_0)) \neq 0$ , we obtain that  $u^*$  satisfies the Hamiltonian maximization condition (2.4) as desired as well as the pointwise convergence of  $(u_k)$  to  $u^*$  at every point  $t_0 \in [0, T]$  such that  $\phi(t_0) \neq 0$ . This concludes the proof of the convergence of the sequence of controls  $(u_k)$  to  $u^*$ .

Finally, let us check that  $u^*$  is an optimal solution to (OCP). Doing so, observe that

$$\psi(x_k(T)) \le \psi(\tilde{x}_k(T)),$$

for every admissible pair  $(\tilde{x}_k, \tilde{u})$  of (OCP). Note also that  $\tilde{u}$  is a fixed control in  $\mathcal{U}$ . So, again using Gronwall's Lemma, we can check that  $(\tilde{x}_k)$  strongly-weakly converges to  $\tilde{x}$  over [0, T] where  $\tilde{x}$  is the unique solution to  $\dot{x}(t) = f(\tilde{x}(t)) + u(t)g(\tilde{x}(t))$ , a.e.  $t \in [0, T]$  together with  $\tilde{x}(0) = x_0$ . Hence, passing to the limit as  $k \to +\infty$  ( $\psi$  being continuous) implies that

$$\psi(x^{\star}(T)) \le \psi(\tilde{x}(T)),$$

for every admissible pair  $(\tilde{x}, \tilde{u})$  to (OCP). This shows that  $u^*$  is an optimal solution to (OCP) which ends the proof of the proposition.

**Remark 2.1.** As a byproduct of the previous proposition, we obtain that the value function associated to  $(OCP_k)$  converges to the value function associated to (OCP). In addition, the control  $u_k$  uniformly converges to  $u^*$  on every segment  $[t_1, t_2]$  such that  $\phi(t) \neq 0$  over  $[t_1, t_2]$ .

## 2.4 Discussion about the employed methodology

Recall that in the present setting, chattering may occur whenever (2.1) is verified or whenever the covector is orthogonal to [g, [f, g]] along a singular arc. So, under one of these two conditions, we propose to introduce a sequence of functions  $(f_k)$  approaching f (see (2.7) and (2.8)) and such that (2.9) is verified for every  $k \in \mathbb{N}$ . The main advantage of considering (OCP<sub>k</sub>) in place of (OCP) is that the behavior of an optimal solution to (OCP<sub>k</sub>) might be simpler to handle. Indeed, as shows Proposition 2.1, one can expect Fuller's phenomenon for an optimal solution to (OCP) involving a singular arc. In contrast, if  $(x_k, p_k, u_k)$  is an extremal of (OCP<sub>k</sub>), then, according to the PMP, the corresponding switching function  $\phi_k$  fulfills:

$$\phi_k(t) = p_k(t) \cdot [f_k, [f_k, g]](x_k(t)) + u_k(t)p_k(t) \cdot [g, [f_k, g]](x_k(t)).$$

We can thus expect that along a singular arc  $p_k(t) \cdot [g, [f_k, g]](x_k(t)) \neq 0$ , so Fuller's phenomenon may not arise. In addition, if Legendre-Clebsch's condition is verified for every  $k \in \mathbb{N}$ , then, we can also expect the occurrence of a singular arc of turnpike type (thus a first-order singular arc without involving an infinite number of switching times, see, e.g., [2]). Hence, for the approximated problem, Fuller's phenomenon may not arise even if Legendre-Clebsch's condition is not verified (in that case, we speak of anti-turnpike [3, 4]). Note that we supposed the terminal time T > 0 fixed, but it can also be free (in that case, we can adapt the previous properties by using classical techniques considering an augmented state, see, e.g., [5]). In the next section, we provide three examples for which an optimal solution contains a second-order singular arc. Doing so, we introduce an explicit sequence of functions  $f_k$  approaching the dynamics such that the associated optimal control problem does not possesses chattering.

## 3 Application to three examples involving chattering

Throughout this section, we are given a sequence  $(\varepsilon_k)$  of positive numbers such that  $\varepsilon_k \downarrow 0$  as  $k \to +\infty$ . By limit problem, we mean the optimal control problem for which  $\varepsilon_k = 0$  (i.e. without perturbation).

## 3.1 A variant of Fuller's problem

## 3.1.1 Presentation of the problem

Let  $\rho, \ell : \mathbb{R} \to \mathbb{R}$  be two smooth functions. Consider the three-dimensional optimal control problem

$$\inf_{u \in \mathcal{U}, T \in \mathbb{R}_+} x_3(T) \quad \text{s.t.} \begin{cases} \dot{x}_1 = x_2, \\ \dot{x}_2 = \rho(x_1) + u(t), \\ \dot{x}_3 = \ell(x_1) + \varepsilon_k x_2^2, \end{cases} \begin{cases} x_1(0) = x_1^0 \in \mathbb{R} \\ x_2(0) = x_2^0 \in \mathbb{R} \\ x_3(0) = 0 \end{cases}; \ x(T) \in C, \tag{3.1}$$

where  $C \subset \mathbb{R}^3$  is a non-empty closed convex subset. Suppose that  $\ell : \mathbb{R} \to \mathbb{R}$  has a unique minimum  $x_1^m$  over  $\mathbb{R}$  such that  $\ell'(x_1^m) = 0$  together with  $\ell''(x_1^m) > 0$ . Without any loss of generality, we may also assume that  $\ell(x_1^m) = 0$  (by translation). Furthermore, assume that  $-\rho(x_1^m) \in [-1, 1]$  (this is required for admissibility of singular arcs).

**Remark 3.1.** Fuller's Problem corresponds to the "limit" case  $\varepsilon_k = 0$  together with  $\rho(x_1) = 0$ ,  $\ell(x_1) = x_1^2$ , and  $C = \{(0,0)\} \times \mathbb{R}$ .

The previous framework encompasses this example setting

$$f(x) := \begin{pmatrix} x_2 \\ \rho(x_1) \\ \ell(x_1) \end{pmatrix} ; g(x) := \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} ; f_k(x) := \begin{pmatrix} x_2 \\ \rho(x_1) \\ \ell(x_1) + \varepsilon_k x_2^2 \end{pmatrix},$$

since we can easily check that [g, [f, g]] = 0 and  $[g, [f_k, g]] = (0, 0, -2\varepsilon_k)^\top \neq 0$  (for  $\varepsilon_k > 0$ ). We now provide more details on optimal solutions of (3.1) for  $\varepsilon_k > 0$  and in the limit case.

1. Study of the optimal control problem in the case where  $\varepsilon_k > 0$ . By application of the PMP considering only normal lifts, the Hamiltonian of the problem becomes:

$$H_k := p_1 x_2 + p_2 \rho(x_1) + p_2 u - \ell(x_1) - \varepsilon_k x_2^2.$$

Indeed, using the transversality condition, we obtain that  $p_3(T) = -1$  and because  $H_k$  does not depend on  $x_3$ , the function  $p_3$  must be constant. It follows that the adjoint equation can be written as:

$$\begin{cases} \dot{p}_1 = -p_2\rho'(x_1) + \ell'(x_1) \\ \dot{p}_2 = -p_1 + 2\varepsilon_k x_2. \end{cases}$$

The switching function is  $p_2$  which satisfies

$$\ddot{p}_2 = p_2 \rho'(x_1) - \ell'(x_1) + 2\varepsilon_k \rho(x_1) + 2\varepsilon_k u.$$

We are now in a position to characterize singular arcs for every  $\varepsilon_k > 0$ . Using that the Hamiltonian is zero along any extremal (since the terminal time is free), every singular arc is such that:

$$\varepsilon_k x_2^2 = \ell(x_1) \; ; \; u_k^{\star} = \frac{\ell'(x_1)}{2\varepsilon_k} - \rho(x_1) \; ; \; \ddot{x}_1 = \frac{\ell'(x_1)}{2\varepsilon_k},$$

where  $u_k^{\star}$  denotes the singular control. The set of points  $(x_1, x_2) \in \mathbb{R}^2$  such that  $\varepsilon_k x_2^2 = \ell(x_1)$  is the singular locus. In addition, for every  $k \in \mathbb{N}$ , we find that  $\ddot{p}_{2|_u} = 2\varepsilon_k > 0$  thus Legendre-Clebsch's condition is verified along a singular arc. In particular, since  $\varepsilon_k \neq 0$ , every singular arc is of first order.

2. Study of the optimal control problem in the limit case. Using similar notation as when  $\varepsilon_k > 0$ , we find that the switching function associated with the optimal control problem with  $\varepsilon_k = 0$  now satisfies

$$\ddot{p}_2 = p_2 \rho'(x_1) - \ell'(x_1),$$

thus, we need to differentiate  $p_2$  at least four times to check the order of the singular control. Note also that we must have  $-\ell'(x_1) = 0$  along a singular arc, hence,  $x_1 = x_1^m$ . By differentiating  $\ddot{p}_2$  w.r.t. t, we find that  $\ddot{p}_2 = -\ell''(x_1)x_2$ , hence  $x_2 = 0$  along the singular arc (because  $\ell''(x_1^m) > 0$ ), and finally  $\ddot{p}_2 = -\ell''(x_1^m)u$ . In that case, a singular arc is then characterized by

$$x_1^{\star} = x_1^m \; ; \; x_2^{\star} = 0 \; ; \; u^{\star} = -\rho(x_1^m),$$

where  $u^{\star}$  is the singular control. We conclude that the limit case has a second-order singular arc which is such that  $\ddot{p}_{2|_{u}} = -\ell''(x_{1}^{m}) < 0$ , thus Legendre-Clebsch's condition is also verified. In addition,  $|u^{\star}| = |-\rho(x_{1}^{m})| \leq 1$ , thus the singular arc is admissible.

**Remark 3.2.** (i) When  $\varepsilon_k > 0$ , the singular arc is of turnpike type, however, a saturation phenomenon may occur since for t > 0, one has  $|u_k^*(t)| \leq 1$  if and only if

$$\left|\frac{\ell'(x_1(t))}{2\varepsilon_k} - \rho(x_1(t))\right| \le 1.$$

Since  $\varepsilon_k$  is small, the singular arc is admissible only if  $x_1$  is close to  $x_1^m$ . This defines a "small" subset of the singular locus in the plane  $(x_1, x_2)$  for the admissibility of the singular arc. We also see that the singular locus as  $\varepsilon_k \downarrow 0$  is a small deformation of the origin (the singular locus for the problem with  $\varepsilon_k = 0$ ).

(ii) Uniform convergence of the sequence  $(f_k)$  and its derivative  $(D_x f_k)$  to f and  $D_x f$  respectively is straightforward over compact subsets of  $\mathbb{R}^3$ . But, since for a given initial condition  $(x_1^0, x_2^0, 0) \in \mathbb{R}^3$ , optimal trajectories of (3.1) are uniformly bounded, the uniform convergence of  $f_k$  to f on compact subsets is enough to apply the results of Proposition 2.2.

In the next section, we depict numerically optimal solutions when  $\varepsilon_k > 0$  and also in the limit case.

#### 3.1.2 Numerical simulations on the perturbed optimal control problem

For all the examples presented in this article, simulations were carried out with the direct method, using the Bocop solver [23]. For sake of simplicity, the final time was fixed. The Gauss II method<sup>3</sup> was used for discretization, with 1000 time steps. Simulations of the perturbed Fuller's problem (*i.e.*, Problem (3.1) with  $\rho(x_1) = 0$  and  $\ell(x_1) = x_1^2$ ) are depicted on Fig. 1 and 2 for different values of  $\varepsilon_k$ . In line with our previous results, the trajectories are of type Bang-Singular. In particular, Fig. 2 highlights the fact that optimal paths (for  $\varepsilon_k > 0$ ) lie in the singular locus  $\varepsilon_k x_2^2 = x_1^2$  before approaching the target point (see Remark 3.2). As  $\varepsilon_k$  decreases, we can see that the number of bang arcs increase and the trajectories approximate that of the original problem. Optimal controls are a succession of bang arcs together with a "small" terminal first-order singular arc such that the optimal path lies in the singular locus and then reaches the target point.

Also, we have performed a numerical simulation of optimal paths when  $\varepsilon_k < 0$ , see Fig. 3. In that case, Legendre-Clesbsch's condition has the opposite sign leading that way to an anti-turnpike behavior. It follows that approximated optimal controls are a succession of bang arcs (see, *e.g.*, [3]). In that case, no singular arcs occurs.

### 3.2 Application to a resource allocation model

## 3.2.1 Presentation of the model

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We consider a control system describing a self-replicator model of bacterial growth where  $x_1$  is the concentration of precursors within a cell and  $x_2$  denotes the concentration of gene expression machinery. The control u with values in [0, 1] will denote the resource allocation parameter defining the proportion of precursors used for making gene expression machinery. The dynamical resource allocation model amounts then to maximize biomass, in order to understand cellular regulations acquired through evolution. For more details on the modeling, we refer to [13]. This yields the three-dimensional Mayer optimal control problem

$$\inf_{\iota(\cdot)\in[0,1]} x_3(T) \quad \text{s.t.} \begin{cases} \dot{x}_1 = e(1-x_2) - (1+x_1)h(x_1, x_2), \\ \dot{x}_2 = h(x_1, x_2)(u(t) - x_2), \\ \dot{x}_3 = -h(x_1, x_2), \end{cases}; \begin{cases} x_1(0) = x_1^0, \\ x_2(0) = x_2^0, \\ x_3(0) = 0, \end{cases}$$
(3.2)

 $<sup>^{3}</sup>$ It is an implicit method of fourth order in two stages to solve numerically an ordinary differential equation, [23].



Figure 1: Simulations of the perturbed Fuller's problem with different values of  $\varepsilon_k$ .



Figure 2: Simulations of the perturbed Fuller's problem with different values of  $\varepsilon_k$ . Left: trajectories in the phase plane. Right: Zoom around the origin. The dashed lines correspond to the singular locus  $\varepsilon_k x_2^2 = x_1^2$ .

where  $h(x_1, x_2) := \frac{x_1 x_2}{K+x_1}$ , e, K are positive constants,  $(x_1^0, x_2^0) \in \mathbb{R}_+ \times [0, 1]$ , and T > 0 is fixed. The objective function in (3.2) represents the biomass to be maximized. We can observe that  $x_2$  is always bounded between 0 and 1 provided that  $x_2^0 \in [0, 1]$ , but, this property does not hold for  $x_1$  (for more details, see [13]).

The expression of h will lead to chattering (see below), making the use of this model and its variants (see



Figure 3: Simulations of the perturbed Fuller's problem with  $\varepsilon_k < 0$ . Note that in that case, Legendre-Clebsch's condition has the opposite sign (*i.e.*,  $\ddot{p}_{2|_u} = 2\varepsilon_k < 0$ ), so, we have an anti-turnpike behavior for the solution to the approximated optimal control problem leading to an increasing number of bang arcs.

e.g. [26, 25]) more complex. A way to avoid this behavior is to make a slight perturbation of the system replacing  $h(x_1, x_2)$  by  $h_{\varepsilon}(x_1, x_2) := \frac{x_1}{K + x_1} \frac{x_2}{1 + \varepsilon x_2}$  (actually, we replace  $x_2 \mapsto x_2$  by  $x_2 \mapsto \frac{x_2}{1 + \varepsilon x_2}$ ). Hereafter, we keep  $\varepsilon$  in place of  $\varepsilon_k$  for convenience. Setting  $\tilde{f}(x_1) := \frac{x_1}{K + x_1}$  and  $g_{\varepsilon}(x_2) := \frac{x_2}{1 + \varepsilon x_2}$ , we can rewrite the above control system as follows:

$$\begin{cases} \dot{x}_1 = e(1-x_2) - (1+x_1)\tilde{f}(x_1)g_{\varepsilon}(x_2), \\ \dot{x}_2 = \tilde{f}(x_1)g_{\varepsilon}(x_2)(u(t) - x_2), \\ \dot{x}_3 = -\tilde{f}(x_1)g_{\varepsilon}(x_2). \end{cases}$$
(3.3)

So, for  $\varepsilon = 0$ , we are in the limit case with chattering (see below) whereas for every  $\varepsilon > 0$ , the optimal synthesis may exhibit singular arcs of order at most 1 (see below). In addition, it is easily seen that

$$|g_{\varepsilon}(x_2) - x_2| = \frac{\varepsilon x_2^2}{1 + \varepsilon x_2} \le \varepsilon \; ; \; |g'_{\varepsilon}(x_2) - 1| \le 3\varepsilon,$$

for every  $\varepsilon \in (0, 1]$  and every  $x_2 \in [0, 1]$ . Hence, the convergence results of the previous section can be applied. We shall now verify the properties related to the occurrence of a singular arc by application of the PMP.

1. Study of the optimal control problem in the cases where  $\varepsilon > 0$ . We apply the PMP with the maximum convention. Observe that the cost to be minimized is  $\Phi(x(T)) := x_3(T)$ , so the terminal adjoint vector is  $p(T) := -\nabla \Phi(x(T)) = (0, 0, -1)$ . It follows that H can be written

$$H = p_1 e(1 - x_2) - p_1 (1 + x_1) \bar{f}(x_1) g_{\varepsilon}(x_2) + p_2 \bar{f}(x_1) g_{\varepsilon}(x_2) (u - x_2) + \bar{f}(x_1) g_{\varepsilon}(x_2) \to \max_{u \in [0,1]} g_{\varepsilon}(x_2) + p_2 \bar{f}(x_1) g_{\varepsilon}(x_1) + p_2 \bar{f}($$

so  $u(t) = \operatorname{sign}(p_2(t))$  except along (possible) singular arcs. Note that the switching function  $\phi$  is  $\phi := p_2 \tilde{f}(x_1) g_{\varepsilon}(x_2)$ , but since  $\tilde{f}(x_1) g_{\varepsilon}(x_2) > 0$ , we will compute the derivatives w.r.t. t of  $p_2$  in place of  $\phi$  for

simplification. Now, the covector fulfills over [0, T] the adjoint equation:

$$\begin{cases} \dot{p}_1 &= p_1 g_{\varepsilon}(x_2)(\hat{f}(x_1) + (1+x_1)\hat{f}'(x_1)) - p_2 \hat{f}'(x_1)g_{\varepsilon}(x_2)(u-x_2) - \hat{f}'(x_1)g_{\varepsilon}(x_2), \\ \dot{p}_2 &= p_1 e + p_1(1+x_1)\tilde{f}(x_1)g_{\varepsilon}'(x_2) - p_2 \tilde{f}(x_1)(g_{\varepsilon}'(x_2)(u-x_2) - g_{\varepsilon}(x_2)) - \tilde{f}(x_1)g_{\varepsilon}'(x_2). \end{cases}$$

Let us now address the occurrence of a singular arc. Doing so, suppose that  $p_2 \equiv 0$  over  $[t_1, t_2]$  where  $[t_1, t_2]$  is a sub-interval of [0, T]. We get  $\dot{p}_2 = 0$  thus

$$p_1(e + (1 + x_1)\tilde{f}(x_1)g'_{\varepsilon}(x_2)) = \tilde{f}(x_1)g'_{\varepsilon}(x_2)$$

We now turn to the computation of  $\ddot{p}_2$  (along  $p_2 = \dot{p}_2 = 0$  over  $[t_1, t_2]$ ). We get:

$$\begin{split} \ddot{p}_2 &= \dot{p}_1[e + (1+x_1)\tilde{f}(x_1)g_{\varepsilon}'(x_2)] + p_1\frac{d}{dt}(e + (1+x_1)\tilde{f}(x_1)g_{\varepsilon}'(x_2)) - \frac{d}{dt}(\tilde{f}(x_1)g_{\varepsilon}'(x_2)) \\ &= [p_1g_{\varepsilon}(x_2)(\tilde{f}(x_1) + (1+x_1)\tilde{f}'(x_1)) - \tilde{f}'(x_1)g_{\varepsilon}(x_2)][e + (1+x_1)\tilde{f}(x_1)g_{\varepsilon}'(x_2)] \\ &+ p_1[\dot{x}_1(\tilde{f}(x_1)g_{\varepsilon}'(x_2) + (1+x_1)\tilde{f}'(x_1)g_{\varepsilon}'(x_2)) + (1+x_1)\tilde{f}(x_1)g_{\varepsilon}''(x_2)\dot{x}_2] \\ &- \tilde{f}'(x_1)g_{\varepsilon}'(x_2)\dot{x}_1 - \tilde{f}(x_1)g_{\varepsilon}''(x_2)\dot{x}_2 \end{split}$$

To compute  $\ddot{p}_{2|_{u}}$  there are two contributing terms (from  $\dot{x}_{2}$ ). We get replacing  $p_{1}$  by its value in the second equality:

$$\begin{split} \ddot{p}_{2|_{u}} &= (1+x_{1})\tilde{f}^{2}(x_{1})g_{\varepsilon}''(x_{2})g_{\varepsilon}(x_{2})p_{1} - \tilde{f}^{2}(x_{1})g_{\varepsilon}''(x_{2})g_{\varepsilon}(x_{2}) \\ &= (1+x_{1})\tilde{f}^{2}(x_{1})g_{\varepsilon}''(x_{2})g_{\varepsilon}(x_{2})\frac{\tilde{f}(x_{1})g_{\varepsilon}'(x_{2})}{e + (1+x_{1})\tilde{f}(x_{1})g_{\varepsilon}'(x_{2})} - \tilde{f}^{2}(x_{1})g_{\varepsilon}''(x_{2})g_{\varepsilon}(x_{2}) \\ &= \frac{-e\tilde{f}^{2}(x_{1})g_{\varepsilon}(x_{2})g''(x_{2})}{e + (1+x_{1})\tilde{f}(x_{1})g_{\varepsilon}'(x_{2})}. \end{split}$$

**Proposition 3.1.** Let  $\varepsilon > 0$  and consider an extremal of the optimal control problem. If a singular arc occurs, then, the Legendre-Clebsch condition is fulfilled.

*Proof.* From the preceding expression of  $\ddot{p}_{2|u}$ , we deduce that along a singular arc, the switching function satisfies

$$\ddot{\phi}_{|_{u}} = \frac{-ef^{3}(x_{1})g_{\varepsilon}(x_{2})^{2}g_{\varepsilon}''(x_{2})}{e + (1 + x_{1})\tilde{f}(x_{1})g_{\varepsilon}'(x_{2})} > 0,$$

since  $g_{\varepsilon}$  is strictly concave, whence the result.

#### 2. Study of the optimal control problem in the limit case. We can rewrite the system as follows

$$\begin{cases} \dot{x}_1 &= e(1-x_2) - (1+x_1)f(x_1)x_2\\ \dot{x}_2 &= \tilde{f}(x_1)x_2(u(t)-x_2),\\ \dot{x}_3 &= -\tilde{f}(x_1)x_2. \end{cases}$$

Again, we apply the PMP with the maximum convention and similarly, the terminal adjoint vector is p(T) = (0, 0, -1). It follows that the Hamiltonian H can be written

$$H = p_1 e(1 - x_2) - p_1 (1 + x_1) f(x_1) x_2 + p_2 f(x_1) x_2 (u - x_2) + f(x_1) x_2 \to \max_{u \in [0, 1]}$$

so  $u(t) = \text{sign}(p_2(t))$  except along (possible) singular arcs. As previously, we shall compute the derivatives of  $p_2$  w.r.t. t in place of the switching function  $\phi := p_2 \tilde{f}(x_1) x_2$  (since  $\tilde{f}(x_1) x_2 > 0$ ). The covector fulfills the adjoint equation over [0, T]:

$$\left\{ \begin{array}{ll} \dot{p}_1 &= p_1 x_2 (\tilde{f}(x_1) + (1+x_1) \tilde{f}'(x_1)) - p_2 \tilde{f}'(x_1) x_2 (u-x_2) - \tilde{f}'(x_1) x_2, \\ \dot{p}_2 &= p_1 (e + (1+x_1) \tilde{f}(x_1)) + p_2 \tilde{f}(x_1) (2x_2 - u) - \tilde{f}(x_1). \end{array} \right.$$

Let us now address the occurrence of a singular arc. Doing so, suppose that  $p_2 \equiv 0$  over  $[t_1, t_2]$  where  $[t_1, t_2]$  is a sub-interval of [0, T]. We get  $\dot{p}_2 = 0$  thus

$$p_1(e + (1 + x_1)\tilde{f}(x_1)) = \tilde{f}(x_1).$$

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We now turn to the computation of  $p_2^{(k)}$ , k = 2, 3, 4 (along  $p_2 = \dot{p}_2 = 0$  over  $[t_1, t_2]$ ). We get replacing  $p_1$ ,  $\dot{p}_1$ , and  $\dot{x}_1$  by their respective value:

$$\begin{split} \ddot{p}_2 &= \dot{p}_1[e + (1+x_1)f(x_1)] + p_1[f(x_1) + (1+x_1)f'(x_1)]\dot{x}_1 - f'(x_1)\dot{x}_1 \\ &= [p_1x_2(\tilde{f}(x_1) + (1+x_1)\tilde{f}'(x_1)) - \tilde{f}'(x_1)x_2][e + (1+x_1)\tilde{f}(x_1)] \\ &+ p_1[\tilde{f}(x_1) + (1+x_1)\tilde{f}'(x_1)][e(1-x_2) - (1+x_1)\tilde{f}(x_1)x_2] \\ &- \tilde{f}(x_1)[e(1-x_2) - (1+x_1)\tilde{f}(x_1)x_2] \\ &= p_1[\tilde{f}(x_1) + (1+x_1)\tilde{f}'(x_1)] - \tilde{f}'(x_1)e \\ &= \Psi(x_1), \end{split}$$

where

$$\Psi(x_1) := \frac{e[\hat{f}^2(x_1) - e\hat{f}'(x_1)]}{e + (1+x_1)\tilde{f}(x_1)}.$$

We deduce that if a singular arc occurs, then it is at least of second order since  $\phi_{|_u} = f(x_1)x_2\ddot{p}_{2|_u} = 0$ , *i.e.*,  $p(t) \cdot [g, [f, g]](x(t)) = 0$  along the singular arc. In addition, we obtain that if a singular arc occurs, then, we have  $p_2 = \dot{p}_2 = \ddot{p}_2 = 0$ , so  $\Psi(x_1) = 0$  which gives  $x_1 = x_1^* := \sqrt{eK}$ . We also obtain  $\ddot{p}_2 = \Psi'(x_1)\dot{x}_1 = 0$ . A computation shows that

$$\Psi'(x_1^{\star}) = \frac{2\sqrt{Kee}}{(2Ke + e\sqrt{Ke} + \sqrt{Ke})(K + \sqrt{Ke})}$$

which is obviously non-zero, hence,  $x_1$  remains constant along the singular arc and, so, the singular arc is at least of second order. Finally, differentiating a last time w.r.t. t yields

$$\ddot{p}_{2} = \Psi(x_{1})\ddot{x}_{1} = \Psi'(x_{1})(-\dot{x}_{2}(e + (1 + x_{1})\tilde{f}(x_{1}))).$$

This gives  $\dot{x}_2 = 0$ , hence  $x_2 = 0$  or  $x_2 = u$ . The case  $x_2 = 0$  implies that  $\dot{x}_1 = e > 0$  in contradiction with the fact that  $\dot{x}_1 = 0$ . So, we can conclude that  $u = x_2$ . Hence, the singular arc can be characterized as:

$$x_1^{\star} = \sqrt{eK} \; ; \; x_2^{\star} := \frac{e}{e + (1 + x_1^{\star})f(x_1^{\star})} = \frac{\sqrt{e}(\sqrt{e} + \sqrt{K})}{1 + e + 2\sqrt{e}\sqrt{K}} \; ; \; u^{\star} = x_2^{\star}.$$

Finally, we get that

$$\ddot{p}_{|_{u}}^{} = -\Psi'(x_1^{\star})(e + (1 + x_1^{\star})f(x_1^{\star}))x_2^{\star}(x_1^{\star}) < 0,$$

hence, Legendre-Clebsch's condition is satisfied.

#### 3.2.2 Numerical simulations on the perturbed optimal control problem

Fig. 4 depicts trajectories obtained for different values of  $\varepsilon_k > 0$ . Following [13], simulations are carried out with a fixed final time, and only the transients until reaching the optimal steady-state are depicted (bang arcs also appear at the end of the simulations, but they are not relevant for the biological problem). The results are similar to those of the Fuller's problem. For  $\varepsilon_k > 0$ , optimal controls are a concatenation of bang arcs together with a terminal singular arc approaching the singular arc in the limit case. A value of  $\varepsilon_k = 0.01$  is enough to obtain an accurate approximation of the optimal trajectory to the original problem.

## 3.3 Application to a quantum control system

#### 3.3.1 Presentation of the problem

Here, we consider an optimal control problem introduced in [19] in which chattering occurs. The model describes the control of a three-level quantum system to be steered from a given initial condition on the unit sphere of  $\mathbb{R}^3$  (denoted by  $\mathcal{S}^1$ ) to the north pole (0,0,1). This yields the following optimal control problem (written in Mayer form):

$$\min_{T \ge 0, \, u \in \mathcal{U}} x_4(T) \quad \text{s.t.} \begin{cases} \dot{x}_1 &= -x_2, \\ \dot{x}_2 &= x_1 - u(t)x_3, \\ \dot{x}_3 &= u(t)x_2, \\ \dot{x}_4 &= \frac{x_1^2}{2}, \end{cases} \text{ and } \begin{cases} (x_1(0), x_2(0), x_3(0), x_4(0)) &\in \mathcal{S}^1 \times \{0\}, \\ (x_1(T), x_2(T), x_3(T), x_4(T)) &\in \{(0, 0, 1)\} \times \mathbb{R}. \end{cases}$$



Figure 4: Simulations of the perturbed resource allocation problem (3.2) with different values of  $\varepsilon_k$ .

As it can be verified, the dynamics of  $(x_1, x_2, x_3)$  is with values in  $S_1$ . We assume for sake of simplicity that  $x_3(t) \ge 0, \forall t \in [0, T]$  (by choosing initial conditions) so that one can reduce the dimension of the system. Thus, we can introduce the following control system:

$$\begin{cases} \dot{x}_1 &= -x_2, \\ \dot{x}_2 &= x_1 - u(t)\sqrt{1 - x_1^2 - x_2^2}, \\ \dot{x}_3 &= \frac{1}{2}x_1^2 + \frac{\varepsilon}{2}x_2^2, \end{cases}$$

proceeding as previously, that is, by adding a small perturbation term in the state  $x_3$ . The optimal control problem then amounts to minimize  $x_3(T)$  w.r.t. the pair (T, u) such that  $x_1(T) = x_2(T) = 0$  starting from some initial condition  $(x_1^0, x_2^0, 0) \in \mathbb{R}^3$  such that  $(x_1^0)^2 + (x_2^0)^2 < 1$ .

1. Study of the optimal control problem in the case where  $\varepsilon > 0$ . In that case, the Hamiltonian associated with the problem can be written (taking into account that  $p_3 = -1$  is constant):

$$H = -p_1 x_2 + p_2 x_1 - u p_2 \sqrt{1 - x_1^2 - x_2^2} - \frac{x_1^2}{2} - \varepsilon \frac{x_2^2}{2} \to \max_{u \in [-1, 1]}$$

and it is conserved over [0, T] (since the problem is autonomous) and also equal to zero (because the terminal time is free). The adjoint equation reads as follows:

$$\begin{cases} \dot{p}_1 &= -p_2 - \frac{ux_1p_2}{\sqrt{1-x_1^2 - x_2^2}} + x_1, \\ \dot{p}_2 &= p_1 - \frac{ux_2p_2}{\sqrt{1-x_1^2 - x_2^2}} + \varepsilon x_2 \end{cases}$$

Now, the switching function is  $\phi := -p_2\sqrt{1-x_1^2-x_2^2}$ , so, it is enough to study the behavior of  $p_2$ . Along a singular arc, we have  $p_2 = \dot{p_2} = 0$ , thus  $p_1 = -\varepsilon x_2$ . Replacing into the Hamiltonian yields the singular locus  $\varepsilon x_2^2 = x_1^2$  in the state space. By differentiating this expression, we obtain the value of the singular control

$$u_{\varepsilon}^{\star} := \pm \frac{(1+\varepsilon)|x_1|}{\varepsilon \sqrt{1-x_1^2-x_2^2}}.$$

We note that the value of  $|u_{\varepsilon}^{\star}|$  may exceed 1, so in that case, we have saturation (see [1]). However, numerical simulations indicate that it is admissible when the trajectory is close to the origin (what can be expected).

Finally, the second order derivative of  $p_2$  satisfies:  $\ddot{p}_{2|u} = -\varepsilon \sqrt{1 - x_1^2 - x_2^2} < 0$ . It follows that Legendre-Clesbsch's condition is satisfied (since  $\phi = -p_2$ ).

2. Study of the optimal control problem in the limit case. In this case, the switching function is also  $\phi = -p_2$ . By differentiating w.r.t. t, we find that  $\dot{\phi} = -p_1 + \frac{ux_2p_2}{\sqrt{1-x_1^2-x_2^2}}$ . Let us examine singular arcs in this case. Supposing that  $\phi = 0$  over some time interval  $[t_1, t_2]$  gives us  $-p_1x_2 - \frac{x_1^2}{2} = 0$ . The equation  $\dot{\phi} = 0$  also implies that  $p_1 = 0$ , hence  $x_1 = 0$ . Along the singular arc, we can write  $\ddot{\phi} = -\dot{p}_1 = x_1$ , thus  $\ddot{\phi} = -\dot{x}_1 = x_2$ , and finally  $\dot{\phi} = -\dot{p}_1 = x_1$ .

and finally 
$$\phi = \dot{x}_2 = x_1 - u\sqrt{1 - x_1^2 - x_2^2}$$
. To conclude this case, we obtain that the singular arc satisfies

$$x_1^{\star} = x_2^{\star} = u^{\star} = 0 ; \ \phi_{|_u} = 0 ; \ \phi_{|_u} = -1 < 0.$$

We can thus conclude that the limit case is indeed a second-order singular arc for which Legendre-Clesbch's condition is verified.

#### 3.3.2 Numerical simulations on the perturbed optimal control problem

The results obtained for the perturbed quantum control system are presented on Fig. 5. Here again, we can see that the number of bang arcs increases as  $\varepsilon_k$  decreases. In addition, the trajectory ends up with a singular arc approaching the singular arc of the limit problem (corresponding to u = 0). This example, like the previous ones, confirms the applicability of the method to various control systems.



Figure 5: Simulations of the perturbed quantum control system with different values of  $\varepsilon_k$ .

# 4 Conclusion and perspectives

In this work, we have studied how to slightly modify optimal control problems involving a second order singular arc in order to obtain a "simpler" optimal control problem whose solutions do not possess chattering. The advantage of these modified optimal control problems is that they are more tractable from a numerical viewpoint since optimal controls involve only a finite number of switching times. The examples we have studied show that we obtain that way a deformation of the singular locus (corresponding to the second-order singular arc) into a "small" singular locus (corresponding to a first-order singular arc). Since approximated optimal controls may involve both singular and bang arcs, our approach somehow differs from other approaches using only a sequence of bang-bang arcs to approach the chattering control. In particular, our methodology allows to apply the PMP on the approximated problem and to obtain that way qualitative properties of the approximated control (like the value of the singular control for the approximated problem). Other applications such as in [15] could be investigated in future works. As well, an interesting question could be to find out if every control system involving a second order singular arc (typically, in our setting, when [g, [f, g]] is identically zero) can be approximated by control systems with a first-order singular arc (for which this Lie bracket is nonzero), and how to determine an approximated system. Additionally, convergence of the singular control (for the approximated problem) to the singular control (for the second order singular arc) could also be addressed in future works.

# Declarations

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