
An Application of PL Continuation Methods to Singular Arcs Problems

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Summary. Among optimal control problems, singular arcs problems are interesting and difficult to solve with indirect methods, as they involve a multi-valued control and differential inclusions. Multiple shooting is an efficient way to solve this kind of problems, but typically requires some a priori knowledge of the control structure. We limit here ourselves to the case where the Hamiltonian is linear with respect to the control u , and primarily use a quadratic (u^2) perturbation of the criterion. The aim of this continuation approach is to obtain an approximate solution that can provide reliable information concerning the singular structure. We choose to use a PL (simplicial) continuation method, which can be more easily adapted to the multi-valued case. We will first present some convergence results regarding the continuation, and then study the numerical resolution of two example problems. All numerical experiments were conducted with the Simplicial package we developed.

1 Introduction

In indirect methods, applying the Pontryagin's Maximum Principle to a problem with singular arcs leads to a Boundary Value Problem with a differential inclusion. We denote this BVP with the following notations, that will be used throughout this paper. Let us denote x the state, p the costate, u the control, and φ the state-costate dynamics. If $y = (x, p) \in \mathbf{R}^n$ (n is thus twice the state dimension) and Γ denotes the set valued map of optimal controls, then one has

$$\text{(BVP)} \begin{cases} \dot{y}(t) \in \Phi(y(t)) = \varphi(y(t), \Gamma(y(t))) & \text{a.e. in } [0, t_f] \\ \text{Boundary Conditions} \end{cases}$$

First, we want to obtain some information regarding the structure of the solutions, ie the number and approximate location of singular arcs. We use for this a perturbation of the original problems by a quadratic (u^2) term, as done for instance in [10]. We will show some convergence properties of this continuation scheme, that are mainly derived from the results in [4] by J.P. Aubin and A. Cellina, and [12] by A.F. Filippov. This continuation method

involves following the zero path of a multi-valued homotopy, which is why we chose a simplicial method rather than a differential continuation method (extensive information about continuation methods can be found in E. Allgower and K. Georg [2, 3], and M.J. Todd [20, 21]). Then we will study the practical path following method, and some of the numerical difficulties we encountered, which led us to introduce a discretized formulation of the Boundary Value Problem. Finally, we use the information from these two continuation approaches to solve the optimal control problems with a variant of the multiple shooting method. We will study in this paper two examples (from [11] and [10]) in parallel, whose similar behaviour indicates that our approach is not too problem-dependant.

1.1 First Example

The first example we consider is a fishing problem described in [11]. The state ($x(t) \in \mathbf{R}$) represents the fish population, the control ($u(t) \in \mathbf{R}$) is the fishing activity, and the objective is to maximize the fishing product over a fixed time interval:

$$(P_1) \begin{cases} \text{Max} \int_0^{10} (E - \frac{c}{x(t)}) u(t) U_{max} dt \\ \dot{x}(t) = rx(t)(1 - \frac{x(t)}{k}) - u(t) U_{max} \\ 0 \leq u(t) \leq 1 \quad \forall t \in [0, 10] \\ x(0) = 70 \cdot 10^6 \quad x(10) \text{ free} \end{cases}$$

with $E = 1$, $c = 17.5 \cdot 10^6$, $r = 0.71$, $k = 80.5 \cdot 10^6$ and $U_{max} = 20 \cdot 10^6$.

First we transform this problem into the corresponding minimization problem with the objective $\text{Min} \int_0^{10} (\frac{c}{x(t)} - E) u(t) U_{max} dt$ (note that the numerical values of the problem are such that we always have $\frac{c}{x(t)} - E < 0$, which corresponds to a positive fishing product). Applying the Maximum Principle of Pontryagin then gives the following hamiltonian system for the state x and costate p :

$$\begin{cases} \dot{x}(t) = r x(t) (1 - \frac{x(t)}{k}) - u(t)U_{max} \\ \dot{p}(t) = \frac{c}{x^2(t)} u(t)U_{max} - p(t) r (1 - \frac{2x(t)}{k}). \end{cases}$$

In terms of the switching function ψ

$$t \in [0, 10] \mapsto \psi(t) = \frac{c}{x(t)} - E - p(t),$$

the Hamiltonian minimization gives the optimal control

$$\begin{cases} u^*(t) = 0 & \text{if } \psi(t) > 0 \\ u^*(t) = 1 & \text{if } \psi(t) < 0 \\ u^*(t) \in [0, 1] & \text{if } \psi(t) = 0. \end{cases}$$

Over a singular arc, the relations $\dot{\psi} = 0$ and $\ddot{\psi} = 0$ give the expression of the singular control (t is omitted for clarity)

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

More precisely, the control actually vanishes in the equation $\dot{\psi} = 0$, so it is necessary to use the second derivative of the switching function. On a side note, these relations also lead to $\dot{x} = \dot{p} = 0$, so the state, costate, and therefore also the control are constant over a singular arc for this problem, which is of course not a general property. Another remark is the important difference of magnitude between the state and costate (about 10^8), which requires the use of a proper scaling.

1.2 Second Example

The second example is the quadratic regulator problem studied by Y. Chen and J. Huang [10]:

$$(P_2) \begin{cases} \text{Min } \frac{1}{2} \int_0^5 (x_1^2(t) + x_2^2(t)) dt \\ x_1(t) = x_2(t) \\ \dot{x}_2(t) = u(t) \\ -1 \leq u(t) \leq 1 \quad \forall t \in [0, 5] \\ x(0) = (0, 1) \quad x(5) \text{ free} \end{cases}$$

We have the state and costate dynamics

$$\begin{cases} \dot{x}_1(t) = x_2(t) \\ \dot{x}_2(t) = u(t) \\ \dot{p}_1(t) = -x_1(t) \\ \dot{p}_2(t) = -p_1(t) - x_2(t) \end{cases}$$

and the following switching function and optimal control:

$$\begin{aligned} \psi(t) &= p_2(t), \\ \begin{cases} u^*(t) = -\text{sign } p_2(t) & \text{if } \psi(t) \neq 0 \\ u^*(t) \in [-1, 1] & \text{if } \psi(t) = 0. \end{cases} \end{aligned}$$

In that case again, the control disappears from the equation $\dot{\psi} = 0$, but the relation $\dot{\psi} = 0$ still gives the singular control $u_{singular}^*(t) = x_1(t)$.

2 Continuation Method: A Quadratic Perturbation

Solving these problems directly by single shooting is not possible due to the presence of singular arcs, so we use a continuation method. Like the approach in [10], we try to regularize these problems with a quadratic ($u^2(t)$) perturbation, and consider the following objectives:

$$\begin{aligned} & \text{Min} \int_0^{10} \left(\frac{c}{x(t)} - E \right) (u(t) - (1 - \lambda)u^2(t)) U_{max} dt, \quad \lambda \in [0, 1], \\ & \text{Min} \frac{1}{2} \int_0^5 (x_1^2(t) + x_2^2(t)) + (1 - \lambda)u^2(t) dt, \quad \lambda \in [0, 1]. \end{aligned}$$

For problem (P_1) , as mentioned before the term $\frac{c}{x(t)} - E$ is always negative, so the minus sign before $(1 - \lambda)u^2(t)U_{max}$ actually results in "adding" a quadratic term, as for problem (P_2) . We then obtain two families of boundary value problems parametrized by λ , denoted by $(BVP_1)_\lambda$ and $(BVP_2)_\lambda$ respectively. The original problems correspond to $\lambda = 1$. For $\lambda = 0$, the problems are much more regular, and can be solved directly by single shooting without any difficulties. The principle of the continuation method is to start from the solution at $\lambda = 0$ to attain $\lambda = 1$, where we have the solution of the original problem. The first idea is to try to solve a sequence of problems $(BVP)_{\lambda_k}$, with a sequence (λ_k) ranging from 0 to 1. However, finding a suitable sequence (λ_k) is often problematic in practice, and here the low regularity of the homotopy (for $\lambda = 1$ especially) led us to rather consider a full path following method. More precisely, if we note S_λ the shooting function related to the parametrized problems, we will follow the zero path of the homotopy $h : (z, \lambda) \mapsto S_\lambda(z)$, from $\lambda = 0$ to $\lambda = 1$. There are two main families of path following methods: Predictor-Corrector methods, which are fast but require that the zero path be C^2 , and the slower but more robust Piecewise Linear methods. In the present case, we have to deal for $\lambda = 1$ with a multi-valued homotopy, which is why we use a simplicial method, whose general principle will be described below.

Remark. From now on, we will use the subscripts $_1$ and $_2$ for notations specific to Problems 1 and 2, and keep unsubscripted notations for the general case.

2.1 Hamiltonian Minimization Properties

We begin with some results concerning the Hamiltonian minimization, that were presented in [14]. We first recall a standard result (in the following we keep the notation $y = (x, p)$, with y of dimension n):

Theorem 1. *Assume that $U \subset \mathbf{R}^m$ is a convex compact set with nonempty interior, and that the Hamiltonian function $H : [a, b] \times \mathbf{R}^n \times U \rightarrow \mathbf{R}$ is continuous and convex with respect to the control u . We note $\Gamma(t, x, p)$ the set of solutions of $\min_{u \in U} H(t, x, p, u)$. Then Γ has nonempty compact convex values.*

Lemma 1. *A compact-valued map G is upper-semicontinuous (in the sense of Berge [5, p.114]) if and only if for all sequence (x_k) that converges to x , $(G(x_k))$ converges to $G(x)$ according to*

$$\forall \epsilon > 0, \exists k_0 > 0 \text{ such that } \forall k > k_0, G(x_k) \subset G(x) + \epsilon B(0, 1),$$

with $B(0, 1)$ standing for the closed unit ball of center 0 and radius 1.

Proof. See [17, p.66]. \square

Recall that a function $f : \mathbf{R}^m \times \overline{\mathbf{R}}$ is said to be inf-compact (in the sense of [19]) if for all $(y, a) \in \mathbf{R}^m \times \mathbf{R}$, the set $\{u \in \mathbf{R}^m : f(u) - (u|y) \leq a\}$ is compact. Here $\overline{\mathbf{R}}$ denotes the extended-real line and $(\cdot|\cdot)$ stands for the usual inner product in \mathbf{R}^m .

Lemma 2. *Let $(f_k)_{k \in \mathbf{N}}$ be proper convex lower-semicontinuous functions defined over \mathbf{R}^m . Assume the following assumptions:*

- (i) $(f_k)_{k \in \mathbf{N}}$ converges pointwisely to f ,
- (ii) $\text{int}(\text{dom} f) \neq \emptyset$,
- (iii) f is inf-compact.

Then,

$$\lim_{k \rightarrow \infty} \inf_{u \in \mathbf{R}^m} f_k(u) = \inf_{u \in \mathbf{R}^m} f(u)$$

and, $\forall \epsilon > 0$, there is $k_0 \in \mathbf{N}$ such that

$$\text{argmin}_{u \in \mathbf{R}^m} f_k(u) \subset \text{argmin}_{u \in \mathbf{R}^m} f(u) + \epsilon B(0, 1) \quad \forall k \geq k_0.$$

Proof. See [19], page I.3.54. \square

Theorem 2. *Consider the same hypotheses as in Theorem 1. Then, Γ has the following convergence property: if (t_k, x_k, p_k) is a sequence that converges to (t, x, p) , then*

- (i) $\inf_{u \in \mathbf{R}^m} H(t_k, x_k, p_k, u) \rightarrow \inf_{u \in \mathbf{R}^m} H(t, x, p, u)$ as $k \rightarrow +\infty$,
- (ii) $\forall \epsilon > 0, \exists k_0 > 0$ s.t. $\forall k > k_0, \Gamma(t_k, x_k, p_k) \subset \Gamma(t, x, p) + \epsilon B(0, 1)$.

Proof. Let (t_k, x_k, p_k) be a sequence that converges to (t, x, p) . We note $f_k(u) = H(t_k, x_k, p_k, u) + \delta(u/U)$ and $f(u) = H(t, x, p, u) + \delta(u/U)$ (where $\delta(u/U) = 0$ if $u \in U$, and $+\infty$ if $u \notin U$). For both example problems, it is clear from the expression of the Hamiltonian (see below) that the (f_k) are convex and lower-semicontinuous. Let us check the assumptions of Lemma 2:

(i) If $u \notin U$, then $f_k(u) = f(u) = +\infty \forall k$; if $u \in U$, then $f_k(u) = H(t_k, x_k, p_k, u)$, and as H is continuous we have $H(t_k, x_k, p_k, u) \rightarrow H(t, x, p, u)$, so $f_k(u) \rightarrow f(u)$.

(ii) One has $\text{int}(\text{dom} f) = \text{int}(U) \neq \emptyset$.

(iii) If $v \in \mathbf{R}^m$ and $a \in \mathbf{R}$, then $\{u \mid H(t, x, p, u) + \delta(u/U) - (u|v) \leq a\} = U \cap \{u \mid H(t, x, p, u) - (u|v) \leq a\}$. This set is compact because it is a closed subset of the compact set $U\mathbf{R}^m$. This shows the inf-compactity of f .

Now Lemma 2 proves the theorem. \square

Corollary 1. *Consider the same hypotheses as in Theorem 1. Then, Γ is upper-semicontinuous (in short, usc).*

Proof. Theorem 1, Lemma 1 and Theorem 2 give this result. \square

Remark. If H is strictly convex, then we have the well-known property (see e.g. [13, Theorem 6.1, p.75] and [6]) that u^* is a continuous function (as Γ is then a continuous function).

Back to the two examples, we have $U_1 = [0, 1]$, $U_2 = [-1, 1]$, and the Hamiltonians are (t is omitted for clarity):

$$H_1(t, x, p, u) = \left(\frac{c}{x} - E\right)(u - (1 - \lambda)u^2)U_{max} + p(rx(1 - \frac{x}{k}) - u U_{max}),$$

$$H_2(t, x, p, u) = \frac{1}{2}(x_1^2 + x_2^2 + (1 - \lambda)u^2) + p_1x_2 + p_2u.$$

Both H_1 and H_2 are continuous, and convex with respect to u (for Problem 1 we can numerically check a posteriori that $\frac{c}{x(t)} - E < 0 \quad \forall t \in [0, 10]$). So for both problems (P_1) and (P_2), Theorem 1 and Corollary 1 apply, thus Γ_1 and Γ_2 are upper-semicontinuous, and non empty compact convex valued. These properties will be useful for the following convergence results concerning the continuation. We can also note that for $\lambda < 1$, both Hamiltonians are strictly convex, thus the optimal control are continuous functions.

2.2 Convergence Properties

The following results were presented in [8], and are primarily derived from the books by J.P. Aubin and A. Cellina [4], and by A.F. Filippov [12], whose notations we will keep. In particular,

$$\begin{aligned} \overline{\text{co}} K &= \text{closed convex hull of } K, \\ M^\delta &= \{m : d(m, M) \leq \delta\}. \end{aligned}$$

Definition 1 ([12]). A function y is called a δ -solution of $\dot{y}(t) \in F(t, y(t))$, with $F : [a, b] \times \mathbf{R}^n \rightarrow \mathbf{R}^n$ an upper-semicontinuous set-valued map, if over an interval $[a, b]$, y is absolutely continuous and

$$\dot{y}(t) \in F_\delta(t, y(t)) = [\overline{\text{co}} F(t^\delta, y^\delta)]^\delta$$

where $F(t^\delta, y^\delta) = \cup_{s \in t^\delta, z \in y^\delta} F(s, z)$.

Lemma 3. Let (y_k) be a sequence in $AC_n([a, b])$ such that:

- (i) $\forall t \in [a, b]$, $\{y_k(t)\}_k$ is relatively compact,
- (ii) $\exists l$ such that $|\dot{y}_k(t)| \leq l$ almost everywhere in $[a, b]$.

Then, there exists a subsequence still noted (y_k) that converges uniformly to an absolutely continuous function $y : [a, b] \rightarrow \mathbf{R}^n$, and for which the sequence (\dot{y}_k) converges weakly- $*$ to \dot{y} in $L_n^\infty([a, b])$.

Proof. The proof follows the principle of the demonstration of Theorem 4, pp. 14-15 in [4]. The sequence (y_k) is equicontinuous as

$$|y_k(t') - y_k(t'')| = \left| \int_{t'}^{t''} \dot{y}_k(t) dt \right| \leq l|t' - t''|.$$

The Arzelá-Ascoli theorem implies the existence of a subsequence, still noted (y_k) , that converges uniformly to y in $C_n([a, b])$. Moreover, $\dot{y}_k \in \overline{B}(0, c) \subset$

$L_n^\infty([a, b])$, with $L_n^\infty([a, b])$ being the dual of $L_n^1([a, b])$. Thus the Alaoglu theorem implies that this closed ball is weak-* compact. As $L_n^1([a, b])$ is separable this closed ball is metrizable for the weak-* topology (cf [7]). Then there exists a subsequence, still noted (y_k) , that converges weakly-* to z in $L_n^\infty([a, b])$. We now have to prove that y is absolutely continuous and that $\dot{y} = z$. First, y_k is absolutely continuous, thus

$$y_k(t') - y_k(t'') = \int_{t'}^{t''} \dot{y}_k(s) ds. \tag{1}$$

The sequence (y_k) converges uniformly to y , so the left hand side converges to $y(t') - y(t'')$. As (\dot{y}_k) converges weakly-* to z , for all components i we have

$$\langle \mathbf{1}, \dot{y}_{k,i} \rangle_{L^1, L^\infty} = \int_a^b \dot{y}_{k,i}(s) ds \rightarrow \langle \mathbf{1}, z_i \rangle_{L^1, L^\infty} = \int_a^b z_i(s) ds$$

(where $\mathbf{1}$ is the constant map equal to 1). So the right hand side of (1) converges to $\int_{t'}^{t''} z(s) ds$. We have then

$$y(t') - y(t'') = \int_{t'}^{t''} z(s) ds$$

with z in $L_n^\infty([a, b])$, thus in $L_n^1([a, b])$. This means that y is absolutely continuous and that $\dot{y}(t) = z(t)$ almost everywhere. \square

Theorem 3. *Let (y_k) be a sequence in $AC_n([a, b])$ that converges to y and verifies $\dot{y}_k(t) \in K$ for all k and t , with K compact. Then y is absolutely continuous and $\dot{y}_k(t) \in \overline{\text{co}} K$ for all t .*

Proof. The proof is based on Filippov’s Lemma 13, p. 64 of [12]. \square

Theorem 4. *Let F be a nonempty compact convex valued map, defined on an open set $\Omega \subset \mathbf{R}^{n+1}$. Let (y_k) be a sequence of δ_k -solutions defined on $[a, b]$ that converges uniformly to $y : [a, b] \rightarrow \mathbf{R}^n$ when $\delta_k \rightarrow 0$, and such that the graph of y is in Ω . Then y is a solution of the differential inclusion $\dot{y}(t) \in F(t, y(t))$.*

Proof. See Filippov’s Lemma 1, p. 76 of [12] \square

Lemma 4. *Let $\varphi : \Omega \times [0, 1] \rightarrow \mathbf{R}^n$, with Ω an open subset of \mathbf{R}^n , be a set-valued map verifying*

- (i) φ is upper-semicontinuous with nonempty compact convex values,
- (ii) $\varphi_\lambda = \varphi(\cdot, \lambda)$ is a piecewise $-C^1$ function for $0 \leq \lambda < 1$.

Let us assume that the solutions of $\dot{y}_\lambda(t) = \varphi_\lambda(y(t))$ remain in a fixed compact K and are defined on an interval $[0, t_f]$. Then y_λ is a δ -solution of the differential inclusion $\dot{y}(t) \in \varphi(y(t), 1)$, and δ tends to 0 when $\lambda \rightarrow 1$.

Proof. φ is usc at $(y^*, 1)$ for all $(y^*, 1) \in K$, thus for $\epsilon = \delta$, there exists η such that for all $|y - y^*| < \eta_{y^*} < \delta$, $|\lambda - 1| < \eta_{y^*} < \delta$, we have $\varphi_\lambda(y, \lambda) \in \varphi(y^*, 1)^\epsilon$. Thus $K \subset \cup_{y^* \in K} B(y^*, \eta_{y^*})$ and as K is compact, we have $K \subset \cup_{i=1}^q B(y_i, \eta_i)$. For $\epsilon = \delta, \forall y_i, \exists \eta_i |y - y_i| < \eta_i < \delta$ and $|\lambda - 1| < \eta_i < \delta$, $\varphi_\lambda(y) \in \varphi(y_i, 1)^\epsilon$. For all $y \in K$, there exists y_i such that $y \in B(y_i, \eta_i)$ and thus

$$\varphi_\lambda(y) \in (\varphi(y_i, 1))^\epsilon \subset (\varphi(y_i^\eta, 1))^\epsilon \subset (\varphi(y^\delta, 1))^\epsilon.$$

Then for all λ such that $|\lambda - 1| < \eta$ and for all $y \in K$, we have $\varphi_\lambda(y) \in (\varphi(y^\delta, 1))^\delta$. \square

Theorem 5. *Let us assume that the solutions of $(BVP)_\lambda$ remain in a fixed compact of $[0, t_f] \times K$, $K \subset \Omega$, with Ω an open subset of \mathbf{R}^n . Then from any sequence (y_{λ_k}) of solutions of $(BVP)_{\lambda_k}$, such that $\lambda_k \rightarrow 1$ as $k \rightarrow +\infty$, we can extract a subsequence (y_k) verifying:*

- (i) (y_k) converges uniformly to y solution of $(BVP)_1$,
- (ii) (\dot{y}_k) converges weakly-* to \dot{y} in $L_n^\infty([0, t_f])$.

Proof. φ is usc, thus $\varphi(K, [1 - \epsilon, 1])$ is compact. There exists l such that $|\dot{y}_\lambda(t)| < l$ for $\lambda \in [1 - \epsilon, 1]$. The y_λ are absolutely continuous, and Lemma 3 says that we can extract a subsequence (y_k) that converges uniformly to y , and such that (\dot{y}_k) converges weakly-* to \dot{y} in $L_n^\infty([0, t_f])$. As per Lemma 4, (y_k) is a δ_k -solution. $\varphi(y, 1)$ is non empty compact convex valued, so Theorem 3 says that y is a solution of the differential inclusion $\dot{y}(t) \in \varphi(y(t), 1)$. Initial and terminal conditions can be written as $h_0(y(0)) = 0$ and $h_f(y(t_f)) = 0$ with h_0 and h_f continuous. The uniform convergence of (y_k) implies that y verifies the boundary conditions, thus y is a solution of $(BVP)_1$. \square

Corollary 2. *Under the hypotheses of Theorem 5, assume that $\dot{x} = f(t, x, u)$ provides a control of the form $u = S(t, x) + R(t, x)\dot{x}$, with R and S continuous and R linear. Consider the subsequence $y_k = (x_k, p_k)$ from Theorem 5, and let $u_k = S(t, x_k) + R(t, x_k)\dot{x}_k$. Then (u_k) converges weakly-* in $L_n^\infty([0, t_f])$.*

Proof. See [9], proof of Proposition 3.2, pp. 551-552. \square

Back to our families of problems $(BVP_1)_\lambda$ and $(BVP_2)_\lambda$, we have the state-costate dynamics

$$\varphi_1(y(t), u(t), \lambda) = \left(\begin{array}{c} r x(t) \left(1 - \frac{x(t)}{k}\right) - u(t)U_{max} \\ \frac{c}{x^2(t)} (u(t) - (1 - \lambda)u^2(t))U_{max} - p(t) r \left(1 - \frac{2x(t)}{k}\right) \end{array} \right),$$

$$\varphi_2(y(t), u(t), \lambda) = \begin{pmatrix} x_2(t) \\ u(t) \\ x_1(t) \\ x_2(t) \end{pmatrix}.$$

We consider the set valued dynamic $\Phi(y(t), \lambda) = \varphi(y(t), \Gamma(y(t)), \lambda)$. From the expression of φ_1 and φ_2 , and the fact that Γ_1 and Γ_2 are usc with nonempty

compact convex values, we obtain that Φ_1 and Φ_2 are also usc with nonempty compact convex values. Now we make the assumption that the solutions of $(BVP_1)_\lambda$ and $(BVP_2)_\lambda$ remain in some fixed compact sets, which has been validated by the numerical experiments. Then Theorem 5 applies and gives the convergence result for the continuation approach.

Moreover, we have the following expression of the control:

$$\begin{cases} u_\lambda(t) = \frac{1}{U_{max}}(r x_\lambda(t) (1 - \frac{x_\lambda(t)}{k}) - \dot{x}_\lambda(t)) & \text{for Problem 1} \\ u_\lambda(t) = \dot{x}_{2\lambda}(t) & \text{for Problem 2.} \end{cases}$$

Thus Corollary 2 applies and gives the convergence for the control.

2.3 PL Continuation - Simplicial Method

We will here recall very briefly the principle of a PL continuation method. Extensive documentation about path following methods can be found in E. Allgower and K. Georg [2, 3], as well as Todd [20, 21], to mention only a few. The idea of a continuation is to solve a difficult problem by starting from the known solution of a somewhat related, but easier problem. By related we mean here that there must exist an application h , called a *homotopy*, with the right properties connecting the two problems. For the following definitions we consider that h is a function, the multi-valued case will be treated afterwards.

PL continuation methods actually follow the zero path of the homotopy h by building a piecewise linear approximation of h , hence their name. Towards this end, the search space is subdivided into cells, most often in a particular way called a *triangulation* in *simplices*. This is why PL continuation methods are often referred to as simplicial methods. The main advantage of this approach is that it puts extremely low requirements on the homotopy h : as no derivatives are used, continuity is in particular sufficient, and should not even be necessary in all cases.

First, we recall some useful definitions.

Definition 2. A *simplex* is the convex hull of $n+1$ affinely independent points (called the *vertices*) in \mathbf{R}^n , while a k -*face* of a simplex is the convex hull of k vertices of the simplex (note: k is typically omitted for n -faces, which are just called *faces*).

Definition 3. A *triangulation* is a countable family T of simplices of \mathbf{R}^n verifying:

- The intersection of two simplices of T is either a face or empty,
- T is locally finite (a compact subset of \mathbf{R}^n meets finitely many simplices).

Definition 4. We call *labeling* a map l that associates a value to the vertices v_i of a simplex. We label here the simplices by the homotopy h : $l(v^i) = h(z^i, \lambda^i)$, where $v^i = (z^i, \lambda^i)$. Affine interpolation on the vertices thus gives a PL approximation h_T of h .

Definition 5. A face $[v_1, \dots, v_n]$ of a simplex is said completely labeled iff it contains a solution v_ϵ of the equation $h_T(v) = \epsilon$ for all sufficiently small $\epsilon > 0$ (where $\epsilon = (\epsilon, \dots, \epsilon^n)$).

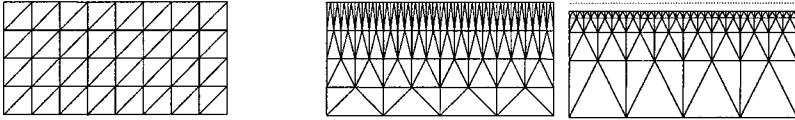


Fig. 1. Illustration of some well known triangulations of $\mathbf{R} \times [0, 1]$ ($[0, 1[$ for J_3): Freudenthal’s uniform K_1 , and Todd’s refining J_4 and J_3

Lemma 5. Each simplex possesses either zero or exactly two completely labeled faces (being called a transverse simplex in the latter case).

Proof. See [2], Chapter 12.4. \square

The constructive proof of this property, which gives the other completely labeled face of a simplex that already has a known one, is often referred to as PL step, linear programming step, or lexicographic minimization. Then there exists a unique transverse simplex that shares this second completely labeled face, that can be determined via the pivoting rules of the triangulation.

A simplicial algorithm thus basically follows a sequence of transverse simplices, from a given first transverse simplex with a completely labeled face at $\lambda = 0$, to a final simplex with a completely labeled face at $\lambda = 1$ (or $1 - \epsilon$ for some refining triangulations that never reach 1, such as J_3), which contains an approximate solution of $h(z, 1) = 0$.

For a multi-valued homotopy h , we have the following convergence property.

Theorem 6. We consider a PL continuation algorithm using a selection of h for labeling and a refining triangulation of $\mathbf{R}^n \times [0, 1[$ (such as J_3 for instance). We make two assumptions regarding the path following:

(i) all the faces generated by the algorithm remain in $K \times [0, 1]$, with K compact.

(ii) the algorithm does not go back to $\lambda = 0$.

Then, if h is usc with compact convex values, the algorithm generates a sequence (z_i, λ_i) such that $\lambda_i \rightarrow 1$, and there exists a subsequence still noted (z_i, λ_i) converging to $(z, 1)$ such that $0 \in h(z, 1)$.

Proof. The proof comes from [1], chapter 4, page 56. \square

For the two examples under consideration, the two assumptions concerning the path following are numerically verified for both problems. However, the assumption of the homotopy convexity only holds for Problem 1, but not for Problem 2 a priori.

2.4 Path Following - Singular Structure Detection

In order to initialize the continuation, we need to solve both problems for $\lambda = 0$, which is easily done by single shooting from an extremely simple initial point ($x(0) = -0.1$ and $x(0) = (0, 0)$ respectively). The objective shown is the original, unperturbed criterion, and the results are summarized on Table 1. For both examples, the path following goes smoothly at first, and the switching function and control evolution as λ increases is quite interesting, as shown on Figures 2 and 3.

Table 1. Solutions for $\lambda = 0$

	λ	z^*	$ S_0(z^*) $	objective	iter	time
Problem 1	0	$-4.0935 \cdot 10^{-2}$	$3.6295 \cdot 10^{-16}$	69374046	39	$< 1s$
Problem 2	0	(1.2733, 2.2715)	$3.3596 \cdot 10^{-14}$	0.4388	134	$< 1s$

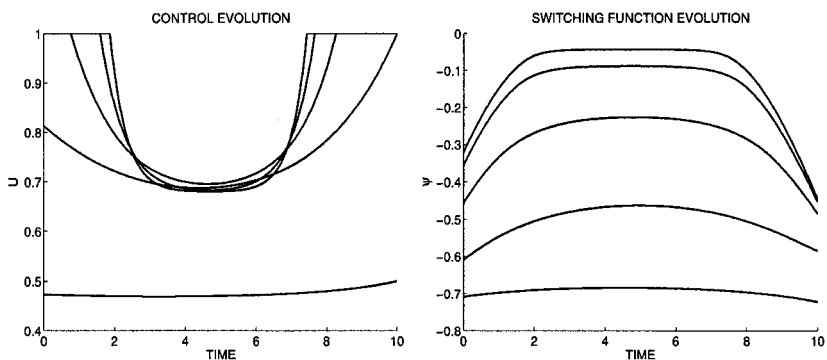


Fig. 2. Problem 1: Control and Switching function for $\lambda = 0, 0.5, 0.75, 0.9, 0.95$

We can see that for both problems, the switching function ψ comes closer to 0 over some time intervals, which strongly suggests the presence of singular arcs at the solution for $\lambda = 1$. For the first problem, the control structure seems to be *regular-singular-regular*, with the singular arc boundaries near $[2, 7.5]$, and for the second problem *regular-singular*, the singular arc beginning around 1.5. Meanwhile, we can see that outside the suspected singular arcs the control tends to a bang-bang structure coherent with the necessary conditions, more precisely +1 before and after the arc for the first problem, and -1 before the arc for the second problem. An interesting fact is that the control keeps on taking intermediate values over the time intervals where ψ tends to 0, which confirms the assumption of a singular arc. On these two examples, the continuation based on the quadratic perturbation gives a strong

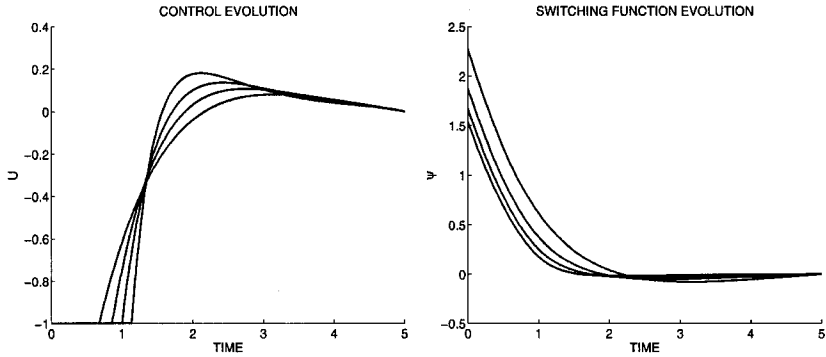


Fig. 3. Problem 2: Control and Switching function for $\lambda = 0, 0.5, 0.75, 0.9$

indication about the control structure, with an approximate location of the singular arcs. So as far as the detection of the singular structure is concerned, this approach seems rather effective.

2.5 Numerical Difficulties - Different Control Structures

However, as λ tends to 1, the path following encounters some difficulties: above a certain point, the PL approximation of the shooting function becomes increasingly inaccurate. We can also note that from this point on, the objective value does not improve any longer (here again, the objective values displayed correspond to the original non-perturbed problems, thus $\text{Max} \int_0^{10} (E - c/x(t)) u(t) U_{\max} dt$ and $\text{Min} \frac{1}{2} \int_0^5 (x_1^2(t) + x_2^2(t)) dt$). Fig.4 shows the evolution of the homotopy norm and the criterion value along the zero path.

Difficulties are often expected at the end of continuation strategies, and for simplicial methods there exists for instance some refining triangulations (such as J_3 or J_4) whose meshsize decreases progressively, in order to ensure an accurate path following near the convergence. Yet in our case, using this kind of techniques only delays this degradation a little, and does not prevent it from appearing eventually. The instability threshold is problem dependant: it appears at best (via refining triangulations) beyond $\lambda = 0.975$ for Problem 1 and $\lambda = 0.95$ for Problem 2.

The reason behind this phenomenon can be found if one looks at the control structures corresponding to the vertices of the completely labeled faces (which are supposed to contain a zero of the PL approximation of the shooting function). Depending on the vertices, we find two different control structures: the interval on which the switching function is close to 0, that we call a *pseudo singular arc*, is not stable. At some point, the switching function leaves the proximity of 0 and increases in absolute value, either with positive or negative

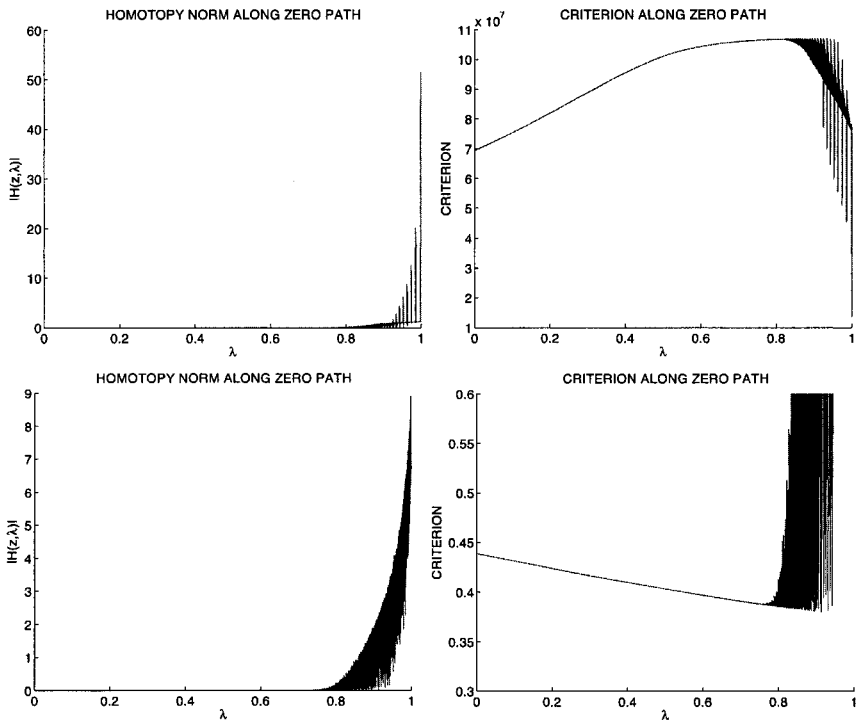


Fig. 4. Homotopy norm and objective value along zero paths, for Problem 1 and 2

sign. Depending on the sign of the switching function at the exit of the pseudo singular arc, we obtain two different control structures, either with “crossing” or “turning back”. What happens is that these two structures keep appearing among the vertices of the labeled faces, however small a meshsize we use, which is why refining triangulations are useless. We also note that this instability of the switching function near zero becomes worse as λ tends to 1: the length of the pseudo singular arc decreases as the exit occurs earlier and earlier, as illustrated on Fig.5.

At the convergence for $\lambda = 1$, all that is left from the pseudo singular arc is a contact point, once again with two possible control structures depending on the sign of the switching function after it reaches 0. For both problems, the control and switching functions (but also the state and costate) are identical for the two structures before the contact point. After that point, which corresponds to the beginning of the supposed singular arc, the switching function goes either positive or negative, with the two corresponding bang-bang controls. More precisely, if the switching function crosses 0 and changes sign, there is a control switch, while it remains the same if the switching function turns back with the same sign after the contact point. Anyway, in both cases

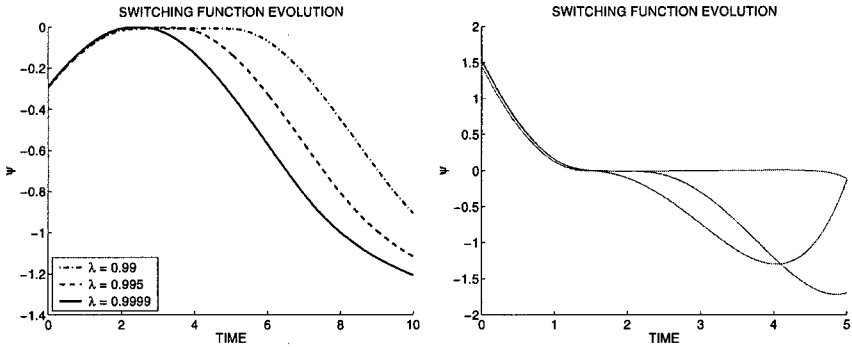


Fig. 5. Switching function evolution for Problem 1 and 2 ($\lambda = 0.99, 0.995, 0.9999$, and $\lambda = 0.95, 0.975, 0.9999$ respectively)

we have lost the singular structure at the convergence. Figures 6 and 7 show these two distinct control structures for each problem.

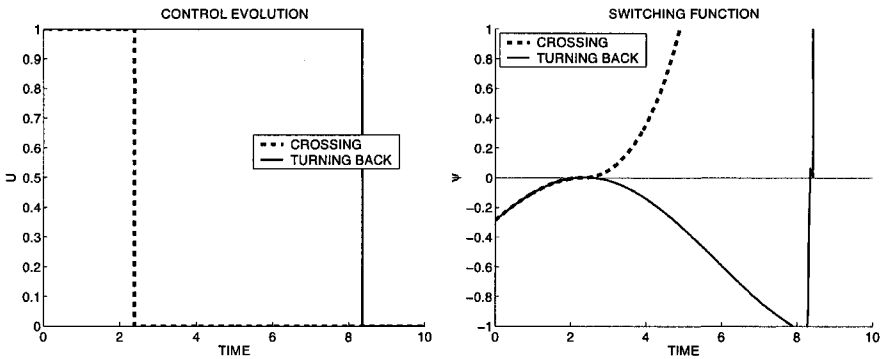


Fig. 6. Problem 1: Control structures according to switch exit sign

The existence of these two very close (with respect to the shooting function unknown z) and yet completely different control structures corresponds to a discontinuity of the shooting function at the solution, which is illustrated on Fig.8 for both Problem 1 (first graph) and Problem 2 (second and third graphs).

We use here a basic Runge Kutta 4th order method with 1000 integration steps. We tried various other fixed step integration methods, such as Euler, Midpoint, Runge Kutta 2 or 3, and increased the number of steps to 10000. We also used variable step integrators, namely Runge Kutta Fehlberg 4-5, Dormand Prince 8-5-3, and Gragg Bulirsch Stoer extrapolation method (see [15]), with similar results.

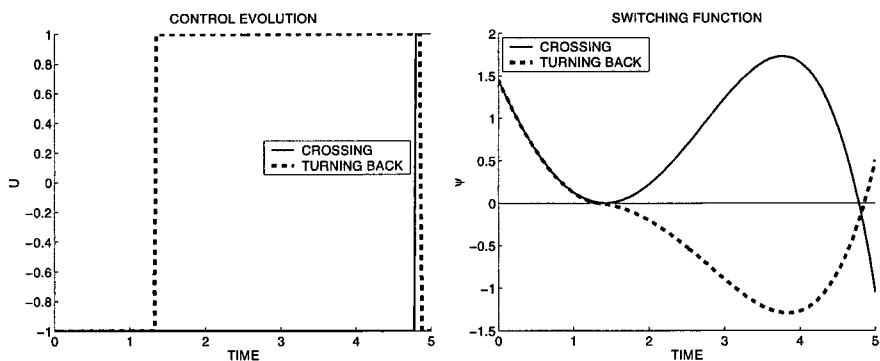


Fig. 7. Problem 2: Control structures according to switch exit sign

For Problem 1, the path following always converges to the correct z^* and locates this discontinuity precisely, which is not surprising as Theorem 6 applies. This is not the case for Problem 2, and the experiments indeed show that the path following can converge to different solutions, depending on the integration used. We also note that the convergence is more difficult to attain for Problem 2, as we often had to use the less accurate triangulation J_4 instead of J_3 .

3 Continuation: Discretized BVP Formulation

We now try to circumvent the previously encountered difficulties by discretizing the equations of the Boundary Value Problem. We use here a basic Euler scheme for the state and costate, and consider a piecewise constant control. The values of the state and costate at the interior discretization nodes become additional unknowns of the shooting function, while we have the following matching conditions at these nodes:

$$\begin{cases} x_{i+1} - (x_i + h \frac{\partial x}{\partial t}(t_i, x_i, p_i, u_i^*)) \\ p_{i+1} - (p_i + h \frac{\partial p}{\partial t}(t_i, x_i, p_i, u_i^*)) \end{cases}$$

where the optimal control u_i^* is obtained from (x_i, p_i) by the usual necessary conditions. The idea is, that even if the control obtained on the singular arc is irrelevant, we hope to have a good approximation of the state and costate values. This formulation corresponds to a particular case of multiple shooting, with a 1-step Euler integration between two successive discretization nodes. Thanks to this integration choice, the discretized version of the shooting function is compact convex valued. This allows us to hope a good behaviour of the path following, according to Theorem 6.

Here are the discretized shooting function unknown and value layouts:

$$\text{Unknown } z \quad \boxed{\text{IVP unknown at } t_0} \mid \boxed{(x^1, p^1)} \mid \boxed{(x^2, p^2)} \mid \dots$$

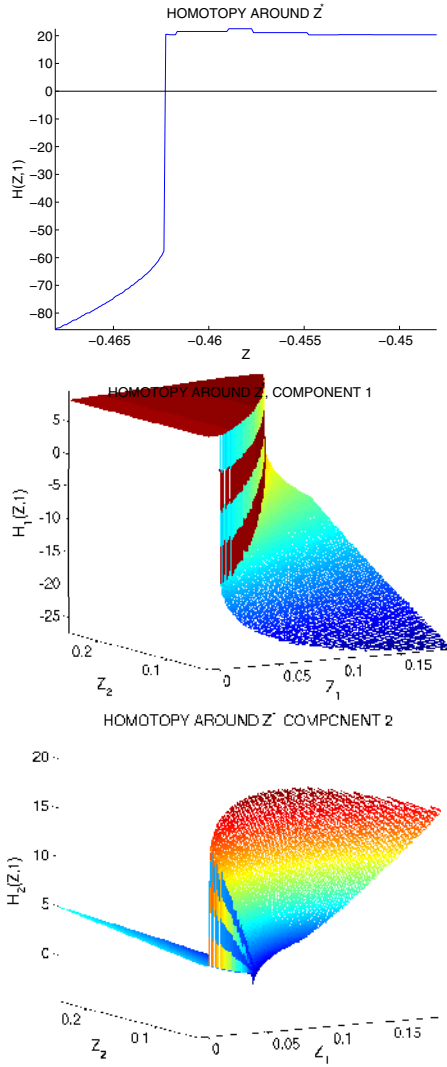


Fig. 8. Shooting functions discontinuity at $\lambda = 1$ for Problem 1 and 2

- IVP unknown at t_0 (same as in single shooting method)
- values of (x^i, p^i) at interior times t_i

$$\text{Value } S_D(z) \quad \boxed{\text{Match}_{cond}(t_1)} \mid \boxed{\text{Match}_{cond}(t_2)} \mid \dots \mid \boxed{\text{Conditions at } t_f}$$

- matching conditions at interior times
- terminal and transversality conditions at t_f (same as single shooting)

Remark. A major drawback of this formulation is that the full state and costate are discretized. This drastically limits the number of discretization nodes, else

the high dimension of the unknown leads to prohibitive execution times. As a side effect, this also puts some restrictions on the use of small meshsizes or refining triangulations, for the same computational cost reasons.

Then we apply the same continuation with the quadratic perturbation as before. Once again, solving both problems for $\lambda = 0$ is done immediately by single shooting, and we follow the zero path until $\lambda = 1$. The instability observed with the single shooting method does not occur. Here on Fig.9 are the solutions obtained with 50 discretization nodes for Problem 1 and 20 for Problem 2 (whose state and costate are in \mathbf{R}^2 instead of \mathbf{R}). This time

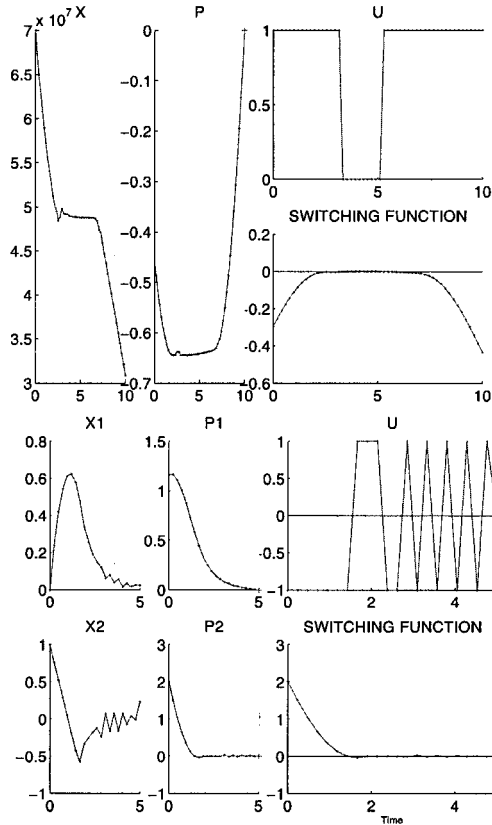


Fig. 9. Discretized BVP solutions at $\lambda = 1$ for Problem 1 and 2

both switching functions clearly show the presence of a singular arc, located near $[2, 7]$ and $[1.5, 5]$ respectively. We note that the switching function for Problem 1 is much closer to zero than the best solution we could obtain with the previous approach. But now, an annoying fact is the presence of some

oscillations located within the bounds of the singular arcs. Trying to get rid of these oscillations by conventional means, such as smaller meshsizes and/or refining triangulations, or increasing the number of discretization nodes, turns out to be ineffective, especially for Problem 2.

These difficulties might come from the expression of the control, which is still given by the necessary conditions. On a time interval $[t_i, t_{i+1}]$ located within a singular arc, let us assume that the continuation has found the correct values of the state and costate (x_i, p_i) and (x_{i+1}, p_{i+1}) . The switching function $\psi(t_i)$ should be near zero as we are supposed to be on a singular arc, but numerically it will not be exactly zero, mostly due to the rough discretization scheme used. The necessary conditions then give a bang-bang control u_i that is different from the actual singular control u_i^* , so the matching conditions on the state and costate at t_{i+1} may not be satisfied. So on singular arcs, the algorithm may deviate to values of (x, p) that try to verify these incorrect matching conditions given by wrong control values.

If we look closer at the value of S_D at the solution, we indeed notice that non-zero components are found only for discretization times corresponding to singular arcs. Moreover, for Problem 2 matching errors only occur for x_2 , whose derivative is the only one in which the control appears. Other components x_1, p_1, p_2 , whose derivatives do not depend on u , always have correct matching conditions, even on the singular arc. For Problem 1, both derivatives of x and p involve the control, so it is not surprising that both matching conditions are non-zero on the singular arc. We also note that the sign of non-zero matching conditions changes accordingly to the sign of the switching function. This is coherent with the fact that it also corresponds to the switchings of the incorrect bang-bang control, and therefore possibly the changes of sign of $u_i - u_i^*$. All this confirms that these oscillations observed on singular arcs are related to the wrong control value given by the necessary conditions. Fig.10 shows these matching conditions, with the switching function.

4 Numerical Resolution

Now we have gathered some knowledge concerning the singular structure of the problems, and we try to solve them more precisely. Based on the solutions of the continuation with the continuous and discretized formulations, we will assume that we have the following control structures: *regular-singular-singular* for Problem 1, and *regular-singular* for Problem 2.

We use a variant of the classical multiple shooting method, that we call “structured shooting”. It shares the same principle as the well known code BNDSCO from H.J. Oberle (see [18]), slightly simplified and adapted to the singular case instead of the state constraints. The control structure is here described by a fixed number of interior switching times, that correspond to the junction between a regular and a singular arc. This times $(t_i)_{i=1..n_{switch}}$ are part of the unknowns and must satisfy some switching conditions. Each

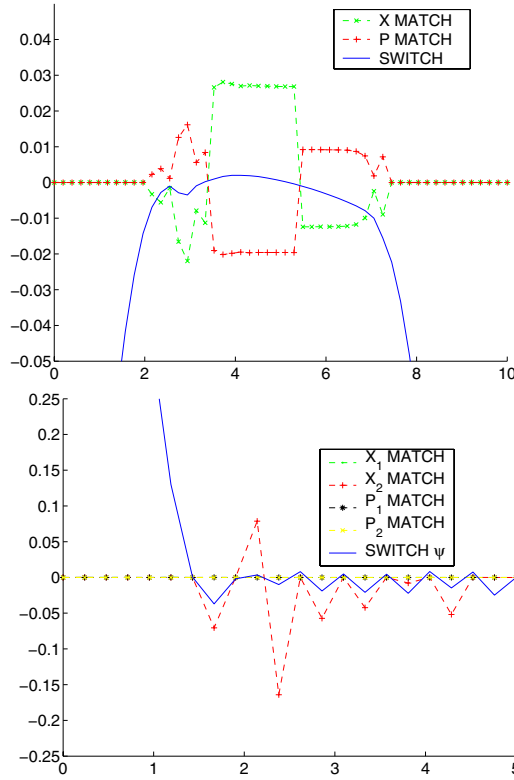


Fig. 10. Matching conditions at $\lambda = 1$ for Problems 1 and 2

control arc is integrated separately, and matching conditions must be verified at the switching times. The switching condition indicates a change of structure, that is the beginning or end of a singular arc where $\psi = 0$, and thus can be defined for instance as $\psi^2(t_i, x_i, p_i) = 0$. Matching conditions basically consist in state and costate continuity at the switching times.

Summary: structured shooting function unknown and value layout:

Unknown z $\boxed{\text{IVP unknown at } t_0} \boxed{(x^1, p^1)} \boxed{(x^2, p^2)} \dots \boxed{\Delta_1} \boxed{\Delta_2} \dots$

- IVP unknown at t_0 (same as in single shooting method)
- values of (x^i, p^i) at interior switching times t_i
- switching times intervals Δ_i , such that $t_i = t_{i-1} + \Delta_i$, $\forall i \in [1..nswitch]$

Value $S_{Struct}(z)$ $\boxed{Switch_{cond}(t_1)} \boxed{Match_{cond}(t_1)} \dots \boxed{\text{Conditions at } t_f}$

- switching and matching conditions at interior times
- terminal and transversality conditions at t_f (same as single shooting)

Structured shooting initialization:

Based upon the solutions obtained with the two continuations, we have two switchings times for Problem 1, and one switching time for Problem 2. The structured shooting unknowns, and the initialization sets corresponding to the continuous and discretized continuations are summarized below on Table 2 and 3 (for the single shooting we use a solution for $\lambda = 0.95$, before instability occurs).

Table 2. Problem 1: control structure regular-singular-regular

Continuation	$p(0)$	$t_1; t_2$	(x^1, p^1)	(x^2, p^2)
$BVP_{0.95}$	-0.429	2.5 ; 7	$(4.996 \cdot 10^7, -0.600)$	$(4.825 \cdot 10^7, -0.587)$
BVP_D	-0.453	2.55 ; 7.06	$(4.839 \cdot 10^7, -0.637)$	$(4.741 \cdot 10^7, -0.621)$

Table 3. Problem 2: control structure regular-singular

Continuation	$(p_1(0), p_2(0))$	t_1	(x^1, p^1)
$BVP_{0.95}$	(0.974, 1.512)	1.5	(0.398, -0.309, 0.401, 0.00358)
BVP_D	(1.167, 2.024)	1.429	(0.578, -0.429, 0.586, 0.000505)

Now we try to solve directly $S_{struct}(z) = 0$ with these initializations. For both problems, convergence is immediate for the two initializations. Fig.11 shows the solutions obtained, with the expected singular arcs. The solutions are the same for the two initialization sets, see Table 4 and 5.

Table 4. Solution comparison for Problem 1 for the two initialization sets.

Initialization	z^*	$t_1^*; t_2^*$	$ S_{Struct}(z^*) $	objective	iter	time
$BVP_{0.95}$	-0.46225	2.3704 ; 6.9888	$1.1 \cdot 10^{-13}$	106905998	110	< 1s
BVP_D	-0.46225	2.3704 ; 6.9888	$3.1 \cdot 10^{-11}$	106905998	88	< 1s

Table 5. Solution comparison for Problem 2 for the two initialization sets.

Initialization	z^*	t_1^*	$ S_{Struct}(z^*) $	objective	iter	time
$BVP_{0.95}$	(0.9422, 1.4419)	1.4138	$2.4 \cdot 10^{-14}$	0.37699	93	< 1s
BVP_D	(0.9422, 1.4419)	1.4138	$9.2 \cdot 10^{-15}$	0.37699	116	< 1s

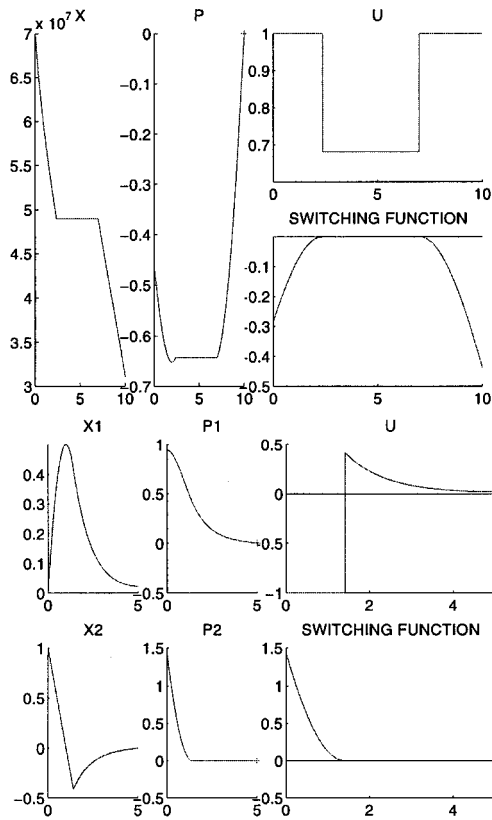


Fig. 11. Solutions obtained by Structured Shooting for Problems 1 and 2

Remark. It should be noted that the resolution can be quite sensitive with respect to the initial point. For Problem 1, a deviation of 0.1 of the costate values can be enough to prevent the convergence.

As a conclusion, we give here a comparison of the solutions obtained by the two continuation approaches (single shooting at $\lambda = 0.95$ and discretized BVP) with the reference solution from structured shooting, see Fig.12 and 13.

We can see that both continuation solutions are rather close to the reference solution for the state, costate and switching function. For Problem 1 the discretized solution is quite good, with very little oscillations, while the continuous solution at $\lambda = 0.95$ is less accurate for p and ψ . For Problem 2, the oscillations are much more important on the discretized solution, whereas the continuous solution at $\lambda = 0.95$ is very close to the reference. Concerning the control, the continuous formulation gives an acceptable approximation of the singular control, the differences being localized around the switching times,

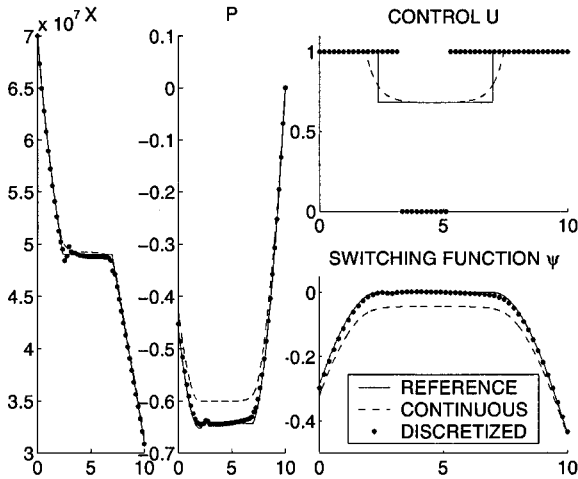


Fig. 12. Structured Shooting and continuation solutions comparison for Problem 1

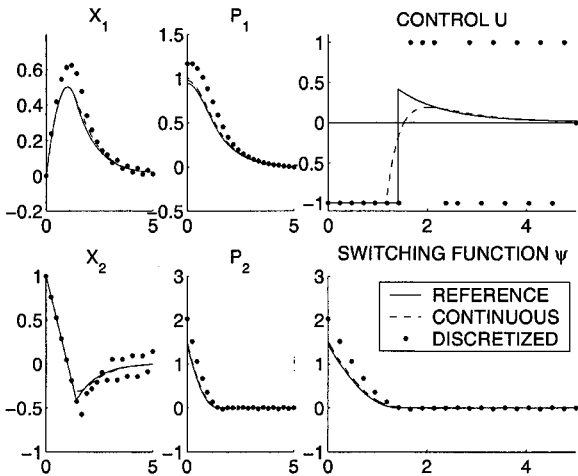


Fig. 13. Structured Shooting and continuation solutions comparison for Problem 2

which is not surprising.

Notes and Numerical precisions:

- There is no path following for structured shooting: we solve $S_{Struct}(z) = 0$ directly, which is possible because we have a quite good initial guess.
- For non-discretized formulations (single and structured shooting), a basic fixed step Runge Kutta 4th order integration was used, with 1000 discretization steps for both problems. As said before, we obtained similar results with

other integration methods, either with fixed or variable step.

- Tests were run on a PC workstation (2.8GHz Pentium 4), using a build of the Simplicial package compiled with ifc (Intel Fortran Compiler).
- All numerical experiments were made using the Simplicial package we wrote, which implements a PL continuation for optimal control problems via indirect methods (www.enseeiht.fr/lima/apo/simplicial/, see also [16])

5 Conclusions and Perspectives

Starting with no a priori knowledge about the control structure, the two formulations (single shooting and discretized BVP) of the continuation allowed us to detect the singular arcs accurately. With this information and the approximate solutions obtained, we were able to solve the problems with a variant of multiple shooting.

Concerning the oscillations encountered with the discretized formulation, one could think of using the expression of the singular control when the switching function is close to 0, instead of the incorrect bang-bang control given by the hamiltonian minimization. However, the solutions obtained depend heavily on the practical implementation of this "close to 0" condition, which can artificially force a singular arc...

Another interesting idea is to discretize the control, in the same fashion as direct shooting (or "semi-direct") methods. This consists in integrating the state and costate with an Euler scheme and a piecewise constant control, whose value on the discretization nodes are part of the unknowns. Some conditions would be enforced on these values, such as satisfying the Hamiltonian minimization in the regular case and the singular control expression in the singular case.

Finally, it would be interesting to try to adapt the methods we used here for singular arcs to the case of state constraints, which also lead to low regularity problems.

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