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# A mixed-binary non-linear programming approach for the numerical solution of a family of singular optimal control problems

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This paper presents a new approach for the efficient and accurate solution of Singular Optimal Control Problems (SOCP). A novel feature of the proposed method is that it does not require a priori knowledge of the structure of the solution. As the first step of this method, the SOCP is converted into a binary optimal control problem. Then, by utilizing the pseudospectral method, the resulting problem is transcribed to a mixed-binary non-linear programming problem. This mixed-binary non-linear programming problem. This mixed-binary non-linear programming problem, which can be solved by well-known solvers, allows us to detect the structure of the original optimal control and to compute the approximating solution of it (getting both the optimal state and control). The main advantages of the present method are that: (i) without a priori information, the structure of optimal control is detected; (ii) it produces good results even using a small number of collocation points; and (iii) the switching times can be captured accurately. These advantages are illustrated through a numerical implementation of the method on four examples.

**Keywords:** Singular optimal control problem; Feedback rule; Legendre-Gauss-Radau pseudospectral method; Mixed-binary non-linear programming

#### 1. Introduction

A classical and challenging subject in the optimal control field is the Singular Optimal Control Problem(SOCP). In these problems, the Pontryagin's maximum principle fails to provide information on the optimal control over at least one interval. SOCPs arise in many areas, ranging from aerospace engineering (Goddard, 1920; Powers & McDanell, 1971) to robotic (Y. Chen & Desrochers, 1993), industrial chemistry (Luus & Okongwu, 1999; Oberle & Sothmann, 1999), biological science (Ledzewicz, Maurer, & Schättler, 2011; Ledzewicz & Schättler, 2008) and other applications (Do Rosário De Pinho, Foroozandeh, & Matos, 2016; L'Afflitto & Haddad, 2016).

The main difficulty in solving SOCPs lies in determining the switching structure of optimal control function, i.e. the sequence of singular and bang-bang sub-arcs and location of switching points (Maurer, 1976). Despite the considerable advances in the development of numerical methods to solve optimal control problems, the solution of SOCPs has remained a challenge due to the switching structure, which is not known a priori. This technical difficulty has been a serious setback for the computation of the solution of SOCPs for both indirect and direct methods. When direct methods are used, the accuracy of the solution of SOCPs, especially in singular arcs, is not satisfactory and the structure of optimal control may not be detected adequately. On the other hand, indirect methods, such as multiple shooting, require a priori knowledge of the optimal control structure and furthermore a good initial guess must be provided not only for the states but also

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for the adjoint variables. Accordingly, the development of new methods for solving SOCPs in an efficient way is highly desirable.

Not surprisingly, the simulation and numerical approximation of SOCPs have received considerable attention. In this respect, we refer the reader to gradient techniques (Pagurek & Woodside, 1968), modified gradient techniques (Soliman & Ray, 1972), quasi Newton algorithm (Edge & Powers, 1976), quasi-linearization technique (Aly & Chan, 1973), indirect multiple shooting method (Aronna, Bonnans, & Martinon, 2013; Maurer, 1976), direct shooting method (Vossen, 2010), iterative dynamic programming method (Luus, 1992), line-up competition algorithm (Sun, 2010) and modified Pseudospectral method (Foroozandeh, Shamsi, Azhmyakov, & Shafiee, 2017). In most of the mentioned papers, the control structure is assumed a priori. However, several authors have proposed methods to detect the structure of optimal control. Among those, we refer to epsilon smoothing methods (Bell & Jacobson, 1975), indirect shooting with epsilon smoothing (Bulirsch, Montrone, & Pesch, 1991) and other relevant methods (Fraser-Andrews, 1989; Szymkat & Korytowski, 2003; Tsygankov, 1999). As another family of methods of interest, we can refer to the two-phase methods which are developed to reduce the drawbacks of the aforementioned methods (Bonnans, Martinon, & Trélat, 2008; Foroozandeh, Shamsi, & Do Rosário De Pinho, 2017; Oberle & Sothmann, 1999; Siburian & Rehbock, 2004).

The pseudospectral methods were initially used in fluid dynamics (Canuto, Hussaini, Quarteroni, & Zang, 1991). Since 1990s, the application of the pseudospectral methods for solving optimal control problems has been popular due to their computational efficiency (Li, 2017; Limebeer, Perantoni, & Rao, 2014; Ross & Karpenko, 2012; Shamsi, 2011). For recent advances in the pseudospectral methods, see, for example, Gong, Ross, and Fahroo (2016); Tang, Liu, and Hu (2016). Pseudospectral methods approximate the state and control variables using interpolating polynomials with specific collocation points such as Legendre-Gauss-Lobatto(LGL), Legendre-Gauss(LG) (Mehrpouya, Shamsi, & Azhmyakov, 2014) and Legendre-Radau(LR) points (Garg et al., 2010). Then, by collocating the state equations and path constraints and using the differentiation matrix, the problem is transcribed to a non-linear programming problem(NLP), which can be solved by the well-developed parameter optimization algorithms. The three most common types of the pseudospectral method are LGL pseudospectral (Elnagar, Kazemi, & Razzaghi, 1995; Fahroo & Ross, 2001), LG pseudospectral (Benson, Huntington, Thorvaldsen, & Rao, 2006) and LR pseudospectral (Garg, 2011; Garg et al., 2010) methods.

It is well-known that pseudospectral methods, especially LR pseudospectral method, provide accurate approximations that converge exponentially when the solution of the problem is smooth (Elnagar et al., 1995; Garg et al., 2010). However, SOCPs are known to have nonsmooth solutions and so the application of the pseudospectral methods can be problematic and high-order accuracy of the method may be deteriorated. Additionally, switching points cannot be captured by these methods. In this respect, it is important to note that adding more nodes to overcome these difficulties may lead to inefficiencies and ill-conditioning of the resulted NLP.

In this paper, we propose a new direct approach for solving SOCPs in an efficient and accurate way. A novel feature of our method is that the control structure is determined automatically. Moreover, our method also captures the switching times with high accuracy.

Our method is based on a modified Legendre-Radau pseudospectral method (Garg et al., 2010) and on Mixed-Binary Non-Linear Programming(MBNLP) (Lee & Leyffer, 2011). We first consider some decision variables as candidates for switching points and then we construct a multi-domain form of SOCP. Next, using feedback law and introducing binary variables, the problem is reformulated into a binary optimal control problem. Finally, the binary optimal control problem is transcribed to an MBNLP by the Legendre-Radau pseudospectral method. By solving the resulted MBNLP, the structure of optimal control and position of switching points of our original problem are provided.

The paper is organized as follows. In Section 2, the formulation of SOCPs and some necessary definitions are reviewed. Section 3 provides some background helpful to understand LR pseudospec-

tral methods. Section 4 is dedicated to the description of our method to solve SOCPs. The proposed method is then applied to four examples in Section 5. In final, a conclusion is given in Section 6.

### 2. Statement of the Problem and Preliminaries

Consider the following optimal control problems in the Mayer form, where the control function appears linearly in the dynamic system

min 
$$\mathcal{J}(\mathbf{x}, \mathbf{u}, t_f) = g(\mathbf{x}(t_0), \mathbf{x}(t_f), t_f),$$
 (1a)

s.t. 
$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t) = \mathbf{f}_1(\mathbf{x}(t), t) + \mathbf{F}_2(\mathbf{x}(t), t)\mathbf{u}(t),$$
 (1b)

$$\boldsymbol{\psi}(\mathbf{x}(t_0), \mathbf{x}(t_f), t_f) = 0, \tag{1c}$$

$$\mathbf{u} \in \mathcal{U}.$$
 (1d)

Here,  $t_f$  may be fixed or free, the state variable  $\mathbf{x}(t) = [x_1(t), \dots, x_p(t)]^T \in \mathbb{R}^p$  is a continuous vector function,  $\mathbf{u}(t) = [u_1(t), \dots, u_q(t)]^T \in \mathbb{R}^q$  is a piecewise continuous vector function and the admissible set of control functions is defined as

$$\mathcal{U} = \left\{ \mathbf{u} \mid u_i^{\min} \le u_i(t) \le u_i^{\max}, \ i = 1, \dots, q \right\}.$$

Furthermore, the functions  $g, \mathbf{f}_1, \mathbf{F}_2$  and  $\boldsymbol{\psi}$  are sufficiently continuously differentiable in all arguments and defined by the following mappings:

$$g: \mathbb{R}^{2p+1} \to \mathbb{R}, \quad \mathbf{f}_1, \mathbf{F}_2: \mathbb{R}^{p+1} \to \mathbb{R}^p, \quad \boldsymbol{\psi}: \mathbb{R}^{2p+1} \to \mathbb{R}^r, \ 0 \le r \le 2p.$$

The Hamiltonian function of the above problem is defined by:

$$\mathscr{H}(\mathbf{x}, \mathbf{u}, \boldsymbol{\lambda}, t) := \boldsymbol{\lambda}^T \mathbf{f}_1(\mathbf{x}, t) + \boldsymbol{\lambda}^T \mathbf{F}_2(\mathbf{x}, t) \mathbf{u},$$
(2)

where  $\boldsymbol{\lambda}(t) = [\lambda_1(t), \dots, \lambda_p(t)]^T \in \mathbb{R}^p$  is the so-called adjoint or co-state vector function.

According to the Pontryagin's minimum principle (Pontryagin, Boltyanskii, Gamkrelidze, & Mishchenko, 1962), the solution of the problem (1) requires minimization of the Hamiltonian function (2) with respect to  $\mathbf{u} \in \mathcal{U}$  along the entire trajectories, which satisfy (1b), (1c) and the following conditions:

$$\dot{\boldsymbol{\lambda}}^{*}(t) = -\mathscr{H}_{\mathbf{x}}(\mathbf{x}^{*}(t), \mathbf{u}^{*}(t), \boldsymbol{\lambda}^{*}, t), \qquad (3)$$

$$\boldsymbol{\lambda}^*(t_0) = -\mathbf{l}_{\mathbf{x}_0}(\mathbf{x}^*(t_0), \mathbf{u}^*(t_f), t_f^*, \boldsymbol{\rho}), \tag{4}$$

$$\boldsymbol{\lambda}^*(t_f) = \mathbf{l}_{\mathbf{x}_f}(\mathbf{x}^*(t_0), \mathbf{u}^*(t_f), t_f^*, \boldsymbol{\rho}),$$
(5)

$$\mathscr{H}(t_f) + \mathbf{l}_{t_f}(\mathbf{x}^*(t_0), \mathbf{u}^*(t_f), t_f^*, \boldsymbol{\rho}) = 0, \text{ if } t_f \text{ is free},$$
(6)

where

$$\mathbf{l}(\mathbf{x}_0, \mathbf{x}_f, t_f, \boldsymbol{\rho}) := g(\mathbf{x}_0, \mathbf{x}_f, t_f) + \boldsymbol{\rho}^T \boldsymbol{\psi}(\mathbf{x}_0, \mathbf{x}_f, t_f).$$
(7)

In the considered problem,  $\mathbf{u}$  appears linearly in the dynamic equations. So, the Hamiltonian is linear in the control  $\mathbf{u}$  as well. The factor associated with  $\mathbf{u}$  in the Hamiltonian is called switching function and denoted by:

$$\boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\lambda}, t) := \boldsymbol{\lambda}^T \mathbf{F}_2(\mathbf{x}, t) = [\sigma_1(\mathbf{x}, t), \dots, \sigma_q(\mathbf{x}, t)].$$
(8)

As a result of Pontryagin's minimum principle, if there exists an interval  $[t_1, t_2] \in [t_0, t_f]$  in which the *j*-th component of the switching function  $\sigma(t)$  is positive (negative), then  $u_j(t)$  takes the smallest (largest) admissible control value  $u_j^{\min}(u_j^{\max})$ . So, if  $\sigma_j(t)$  in the time interval  $[t_1, t_2] \in [t_0, t_f]$  has finite isolated zeros, then the optimal control  $u_j^*(t)$  fulfills:

$$u_j^*(t) \in \{u_j^{\min}, u_j^{\max}\}, \quad \forall t \in [t_1, t_2].$$
 (9)

In this case, the  $u_j$  is called *bang-bang* in the interval  $[t_1, t_2]$ . However, if there is a time interval  $[t_1, t_2] \in [t_0, t_f]$  in which the switching function  $\sigma_j(t)$  vanishes, then the Pontryagin's minimum principle provides no information on how to select  $u_j^*(t)$ . In this case, the problem is said to be *singular*, the interval  $[t_1, t_2]$  is called a *singular interval* and the control over a singular interval is referred to *singular arc* (Lamnabhi-Lagarrigue & Stefani, 1990). It is noted that the optimal control may be singular across the entire interval. In this case, the control function is said to be *entirely (or purely) singular*.

In summary, minimization of the Hamiltonian function leads to the following control law (Kirk, 2012; Pontryagin et al., 1962):

$$u_{j}^{*}(t) = \begin{cases} u_{j}^{\min}, & \text{if } \sigma_{j}(t) > 0, \\ u_{j}^{\max}, & \text{if } \sigma_{j}(t) < 0, \\ u_{j}^{\sin}, & \text{if } \sigma_{j}(t) = 0, \end{cases}$$
(10)

In general, singular optimal control contains both bang-bang and singular sub-arcs. A point  $t \in [t_0, t_f]$  is called a switching point if it is a transition between one bang-bang arc and another bang-bang or singular arc switching point(s).

#### 2.1 Order of singular optimal control problems

For the sake of simplicity, we first focus on SOCPs with scalar control, i.e. q = 1,  $\mathbf{u}(t) = u_1(t)$ and  $\boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\lambda}, t) = \sigma_1(\mathbf{x}, \boldsymbol{\lambda}, t)$ . Clearly,  $\frac{d}{dt} \boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\lambda}, t)$  is explicitly a function of  $\mathbf{x}$ ,  $\boldsymbol{\lambda}$ ,  $\dot{\mathbf{x}}$ ,  $\dot{\boldsymbol{\lambda}}$  and t. By replacing  $\dot{\mathbf{x}}$  and  $\dot{\boldsymbol{\lambda}}$  with (1b) and (3), one can express  $\frac{d}{dt} \boldsymbol{\sigma}(\mathbf{x}, \boldsymbol{\lambda}, t)$  as a function of  $\mathbf{x}$ ,  $\boldsymbol{\lambda}$  and t. According to Lewis (1980), the control function u does not appear in  $\frac{d}{dt}\sigma$ . For j > 1,  $\frac{d^j}{dt^j}\sigma(\mathbf{x}, \boldsymbol{\lambda}, t)$ is also expressed as a function of  $\mathbf{x}$ ,  $\boldsymbol{\lambda}$ , t and possibly u. Furthermore, if u appears in  $\frac{d^j}{dt^j}\sigma$ , then it appears linearly (Lewis, 1980). It is possible that the control u does not appear in  $\frac{d^j}{dt^j}\sigma$  for any j. However, if w is the first integer number, in which u appears in  $\frac{d^w}{dt^w}\sigma$ , then w is always even (Lamnabhi-Lagarrigue, 1987; Lewis, 1980). In the former case, the order of SOCP is defined to be infinite and in the latter case, the integer number  $\kappa = \frac{w}{2}$  is called the order of the singular problem.

**Definition 1** (order of singular problem (Lamnabhi-Lagarrigue, 1987)): The integer number  $\kappa$  is called the order of SOCP (1) when  $2\kappa$  is the lowest order derivative of switching function  $\sigma$  such that u appears explicitly. In other words

$$\frac{d^{2\kappa}}{dt^{2\kappa}}\sigma(\mathbf{x},\boldsymbol{\lambda},t) \equiv e(\mathbf{x},\boldsymbol{\lambda},t) + d(\mathbf{x},\boldsymbol{\lambda},t)u, \qquad d \neq 0.$$
(11)

If u never appears explicitly in the differentiation process, then the optimal control problem is called an infinite-order singular problem.

Let the order of SOCP (1) is  $\kappa$  and  $[t_1, t_2]$  is the singular interval. So, in this interval  $\sigma = 0$  and

using (11), we conclude

$$\frac{d^{2\kappa}}{dt^{2\kappa}}\sigma(\mathbf{x},\boldsymbol{\lambda},t) = 0 = e(\mathbf{x},\boldsymbol{\lambda},t) + d(\mathbf{x},\boldsymbol{\lambda},t)u, \qquad d \neq 0.$$
(12)

Now, by solving the equation (12) for u, we get

$$u = u(\mathbf{x}, \boldsymbol{\lambda}, t) = -\frac{e(\mathbf{x}, \boldsymbol{\lambda}, t)}{d(\mathbf{x}, \boldsymbol{\lambda}, t)}, \quad t \in [t_1, t_2].$$

In summary, if the singularity order of the problem is finite, then the control function u can be expressed as a function of  $\mathbf{x}$ ,  $\boldsymbol{\lambda}$  and t.

In some cases, the right-hand side of Eq. (12) does not depend on  $\lambda$  or  $\lambda$  can be eliminated due to:

$$\frac{d^{j}}{dt^{j}}\sigma(\mathbf{x},\boldsymbol{\lambda},t) \equiv 0, \qquad j = 0,\dots, 2\kappa - 1.$$
(13)

In these cases, in the singular interval  $[t_1, t_2]$ , the control u can be obtained in feedback form, i.e. there is a known function  $u^{\text{sing}} : \mathbb{R} \times \mathbb{R}^p \to \mathbb{R}$  such that

$$u(t) = u^{\operatorname{sing}}(t; \mathbf{x}(t)), \qquad \forall t \in [t_1, t_2].$$
(14)

We now turn to problems with vector-valued control. In these problems, let  $u_j$  has a singular arc and  $w_j$  be the first integer number, in which  $u_j$  appears in  $\frac{d^{w_j}}{dt^{w_j}}\sigma_j$ . According to Krener (1977); Vossen (2010),  $w_j$  is even and  $\kappa_j = \frac{w_j}{2}$  is called the order of singular component  $u_j$ . If such  $w_j$  does not exist, then it is said that the order of singular component  $u_j$  is infinite. If the order of singular control  $u_j$  is finite, then using  $\frac{d^{w_j}}{dt^{w_j}}\sigma_j = 0$ , the control  $u_j$  can be obtained as a function of  $\mathbf{x}, \boldsymbol{\lambda}$  and t in the corresponding singular interval.

In most problems, by using additional conditions such as the generalized Legendre-Clebsch condition (Krener, 1977), we can eliminate the adjoint functions and express the singular arc as a function of just  $\mathbf{x}$ , and t. For more details refer, e.g., to Krener (1977); Michel (1996); Vossen (2010). In other words, if  $u_j$  be singular in  $[t_1, t_2]$ , then it can be obtained in the following feedback form

$$u_j(t) = u_j^{\text{sing}}(t; \mathbf{x}(t)), \qquad \forall t \in [t_1, t_2].$$

$$(15)$$

In this paper, we consider a family of optimal control problems, which is stated with the following assumptions.

**Assumption 1:** It is supposed that "chattering phenomenon" (Zelikin & Borosov, 1991) does not occur, i.e. we consider problems with a finite number of singular arcs and switching points.

**Assumption 2:** We assume that the singularity order of the problem is finite and in the singular arcs, the control function can be obtained in the feedback form (15).

#### 3. Background of Legendre-Gauss-Radau pseudospectral Method

In the pseudospectral methods (Fornberg, 1996), the unknown solution is approximated by interpolating polynomials based on some suitable points. On the other hand, its derivatives are approximated by discrete derivative operators (the differentiation matrix). So, the concepts of interpolation and differentiation matrices are useful to understanding the pseudospectral method.

#### 3.1 Approximation by polynomial interpolation

A function g defined on [-1,1] may be approximated by Lagrange polynomials as:

$$g(\tau) \simeq \sum_{i=0}^{n} g(\xi_i)\ell_i(\tau).$$
(16)

Here,  $\xi_i$ , i = 0, ..., n are distinct points in [-1, 1] and called collocation points. Moreover,  $\ell_i(\tau)$ , i = 0, ..., n are the Lagrange polynomials corresponding to these collocation points, which may be expressed as:

$$\ell_i(\tau) = \prod_{j=0, j \neq i}^n \frac{\tau - \xi_j}{\xi_i - \xi_j}, \quad i = 0, \dots, n,$$

with the Kronecker property:

$$\ell_i(\xi_j) = \delta_{ij} = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j. \end{cases}$$
(17)

It is a well-established fact, that a proper choice of collocation points is crucial in terms of accuracy and computational stability of the approximation (16). As a typically good choice of such collocation points, we refer to the well-known Gauss, Gauss-Lobatto and Gauss-Radau points (Funaro, 1992), which lie on [-1, 1] and are clustered near the endpoints.

In Legendre-Gauss-Radau pseudospectral method for optimal control problems (Garg, 2011), the first *n* nodes are Legendre-Gauss-Radau nodes and the last node is selected as  $\xi_n = +1$ . It is noted that Legendre-Gauss-Radau nodes are the roots of  $P_{n-1}(\tau) + P_n(\tau)$ , where  $P_n(\tau)$  is the well-known Legendre polynomial of degree *n*. No explicit formula of the LGR nodes is known. However, these points can be determined by accurate and stable numerical methods (Gautschi, 2004).

To develop a matrix-oriented method, we express Eq. (16) in the following matrix form:

$$g(\tau) \simeq [\boldsymbol{\phi}(\tau)]^T \mathbf{g},$$

where  $\boldsymbol{\phi}(\tau) = [\ell_0(\tau), \dots, \ell_n(\tau)]^T$  is a (n+1)-dimensional vector function and  $\mathbf{g} = [g(\xi_0), \dots, g(\xi_n)]^T$ .

## 3.2 Differentiation matrix

In the pseudospectral methods, it is crucial to express the derivative  $\dot{g}(\tau)$  in terms of  $g(\tau)$  at the collocation points  $\xi_i$ . This expression can be done by using the so-called *differentiation matrices*.

Let g be a function with a sufficient degree of smoothness and approximated as (16). The first derivative of g can be approximated by:

$$\dot{g}(\tau) \simeq \sum_{i=0}^{n} g(\xi_i) \dot{\ell}_i(\tau).$$

By noting that  $\ell_i(\tau)$  is a polynomial of degree n, we can write

$$\dot{\ell}_i(\tau) = \sum_{j=0}^n \dot{\ell}_i(\xi_j) \ell_j(\tau).$$

Using the above two equations, we get

$$\dot{g}(\tau) \simeq \sum_{i=0}^{n} \sum_{j=0}^{n} \dot{\ell}_i(\xi_j) g(\xi_i) \ell_j(\tau),$$

so, the value of  $\dot{g}(\tau)$  in  $\tau = \xi_j$  can be approximated as:

$$\dot{g}(\xi_j) \simeq \sum_{i=0}^n d_{ij}g(\xi_i),$$

where

$$d_{ij} = \dot{\ell}_i(\xi_j), \quad i, j = 0, \dots, n,$$
 (18)

If we consider  $d_{ij}$  as the (i, j)-th component of a matrix **D**, then **D** is called differentiation matrix (Fornberg, 1996). According to (18), the entries of differentiation matrix **D** are computed by taking the analytical derivative of  $\ell_i(\tau)$  and evaluating it at the collocation points  $\xi_j$  for  $i, j = 0, \ldots, n$ . However, more accurate and stable computational methods to compute these entries can be found in Baltensperger and Trummer (2003); Weideman and Reddy (2000); Welfert (1997).

## 4. Mixed-Binary-Non-Linear-Programming Method

In this section, we introduce a direct method for solving SOCP that is based on Mixed-Binary Non-Linear Programming(MBNLP). The first step is to convert SOCP (1) into a binary optimal control problem. Next, using the Radau pseudospectral method, the binary optimal control problem is transformed into an MBNLP. The solution of this last problem gives us an approximate solution of the original SOCP.

### 4.1 Conversion of SOCP to Binary Optimal Control Problem

Based on Assumption 1, we assume that SOCP (1) has a finite number of switching points. However, the number of switching points is not known. The presented method just needs a guess for the upper bound on the number of switching points. Moreover, if this guess is incorrect, then this incorrect choice can be detected by the results of the method. Details on how to choose this guess will be discussed in Section 4.3.

Let the integer and positive number s be the upper bound on the number of switching points. We consider the decision variables  $t_1, \ldots, t_s$  as candidates for switching points, where  $t_0 \leq t_1 \leq \cdots \leq t_s \leq t_f$ . It is worth noting that, these s variables are candidates for switching points and it does not mean that, the optimal control switch at each one. In fact, we do not consider exactly s switch points, but we consider at most s switches.

The decision variables  $t_1, \ldots, t_s$  break the total domain  $[0, t_f]$  into s + 1 sub-domains, i.e. if we

set  $t_0 = 0$  and  $t_{s+1} = t_f$ , then we have

s.

$$[0, t_f] = [t_0, t_1] \cup [t_1, t_2] \cup \dots \cup [t_s, t_{s+1}],$$
(19)

For  $k = 0, \ldots, s$ , denote the restriction of  $\mathbf{x}(t)$  and  $\mathbf{u}(t)$  in the k-th subinterval  $[t_k, t_{k+1}]$  by  $\mathbf{x}^{[k]}(t) = [x_1^{[k]}(t), \ldots, x_p^{[k]}(t)]^T$  and  $\mathbf{u}^{[k]}(t) = [u_1^{[k]}(t), \ldots, u_q^{[k]}(t)]^T$ , respectively. So, the control and state functions are now expressed as:

$$\mathbf{u}(t) = \begin{cases} \mathbf{u}^{[0]}(t), & t \in [t_0, t_1], \\ \mathbf{u}^{[1]}(t), & t \in [t_1, t_2], \\ \vdots & & \\ \mathbf{u}^{[s]}(t), & t \in [t_s, t_{s+1}], \end{cases}, \quad \mathbf{x}(t) = \begin{cases} \mathbf{x}^{[0]}(t), & t \in [t_0, t_1], \\ \mathbf{x}^{[1]}(t), & t \in [t_1, t_2], \\ \vdots \\ \mathbf{x}^{[s]}(t), & t \in [t_s, t_{s+1}]. \end{cases}$$
(20)

It is worthwhile to note that, in each sub-domain, the *j*-th component of the control function  $\mathbf{u}(t)$  is either singular or takes its maximum value (i.e.  $u_j^{\text{max}}$ ) or minimum value (i.e.  $u_j^{\text{min}}$ ). Based on (19) and (20), the problem (1) is now reformulated to the following multi-domain

Based on (19) and (20), the problem (1) is now reformulated to the following multi-domain minimization problem:

min 
$$\mathcal{J}(\mathbf{x}, \mathbf{u}, t_f) := g(\mathbf{x}^{[0]}(t_0), \mathbf{x}^{[s]}(t_f), t_f),$$
 (21a)

t. 
$$\dot{\mathbf{x}}^{[k]}(t) = \mathbf{f}(\mathbf{x}^{[k]}(t), \mathbf{u}^{[k]}(t), t), t \in [t_k, t_{k+1}], k = 0, \dots, s,$$
 (21b)

$$\mathbf{u}^{\min} \leq \mathbf{u}^{[k]}(t) \leq \mathbf{u}^{\max}, t \in [t_k, t_{k+1}], \ k = 0, \dots, s,$$
 (21c)

$$\psi(\mathbf{x}^{[0]}(t_0), \mathbf{x}^{[s]}(t_f), t_f) = 0,$$
(21d)

$$\mathbf{x}^{[k]}(t_{k+1}) = \mathbf{x}^{[k+1]}(t_{k+1}), \ k = 0, \dots, s-1.$$
(21e)

Note that, Eq.(21e) is considered to guarantee the continuity of state functions at the switching points.

As mentioned previously, in the k-th sub-domain  $[t_k, t_{k+1}]$ , the j-th component of  $\mathbf{u}^{[k]}(t)$  takes its value in  $\{u_j^{\min}, u_j^{\max}, u_j^{\sin}(t; \mathbf{x}^{[k]})\}$ . However, these components should be assigned such that the constraints are satisfied and the objective function is minimized. To achieve this goal, we introduce some binary decision variables and the obtaining of optimal solution are carried over the finding of optimal values of these binary decision variables. For this purpose, in each sub-domain  $[t_k, t_{k+1}], k = 0, \ldots s$ , two vectors  $\boldsymbol{\mu}_1^{[k]}$  and  $\boldsymbol{\mu}_2^{[k]}$  with binary components are considered as follows

$$\boldsymbol{\mu}_{1}^{[k]} = [\mu_{11}^{[k]}, \mu_{21}^{[k]}, \dots, \mu_{q1}^{[k]}]^{T} \in \{0, 1\}^{q}, \quad \boldsymbol{\mu}_{2}^{[k]} = [\mu_{12}^{[k]}, \mu_{22}^{[k]}, \dots, \mu_{q2}^{[k]}]^{T} \in \{0, 1\}^{q}.$$

Then the control function, in this sub-domain, is expressed as

$$u_j^{[k]} = \mu_{j1}^{[k]} u_j^{\min} + \mu_{j2}^{[k]} u_j^{\max} + (1 - \mu_{j1}^{[k]} - \mu_{j2}^{[k]}) u_j^{\text{sing}}(t; \mathbf{x}^{[k]}).$$
(22)

Clearly, if  $\mu_{j1}^{[k]} = 1$  and  $\mu_{j2}^{[k]} = 0$  then  $u_j^{[k]} = u_j^{\min}$ . Similarly, if  $\mu_{j1}^{[k]} = 0$  and  $\mu_{j2}^{[k]} = 1$  then  $u_j^{[k]} = u_j^{\max}$  and if  $\mu_{j1}^{[k]} = 0$  and  $\mu_{j2}^{[k]} = 0$  then  $u_j^{[k]} = u_j^{\sin}$ . It is noted that the case  $\mu_{j1}^{[k]} = 1$  and  $\mu_{j2}^{[k]} = 1$  should not happen, and for avoiding this case, the following conditions are imposed

$$\mu_{j1}^{[k]} + \mu_{j2}^{[k]} \le 1, \quad j = 1, \dots, q.$$
 (23)

Based on (22), the control function  $\mathbf{u}^{[k]}(t)$  can be expressed as follows

$$\mathbf{u}^{[k]}(t) = \boldsymbol{\mu}_1^{[k]} \circ \mathbf{u}^{\min} + \boldsymbol{\mu}_2^{[k]} \circ \mathbf{u}^{\max} + \left(\mathbf{1} - \boldsymbol{\mu}_1^{[k]} - \boldsymbol{\mu}_2^{[k]}\right) \circ \mathbf{u}^{\operatorname{sing}}(t; \mathbf{x}^{[k]}),$$
(24)

where  $\circ$  denotes Hadamard product or element by element multiplication, **1** is a *q*-vector which all of its elements are 1 and

$$\mathbf{u}^{\text{sing}}(t;\mathbf{x}^{[k]}) = \left[ \begin{array}{c} u_1^{\text{sing}}(t;\mathbf{x}^{[k]}(t)) \\ \vdots \\ u_q^{\text{sing}}(t;\mathbf{x}^{[k]}(t)) \end{array} \right].$$

Using (24), we can eliminate the control  $\mathbf{u}^{[k]}$  from the optimal control problem (21) and consequently the following binary optimal control problem is derived

min 
$$\mathcal{J}\left(\mathbf{x}, \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, t_{f}\right) := g\left(\mathbf{x}^{[0]}(t_{0}), \mathbf{x}^{[s]}(t_{f}), t_{f}\right)$$
 (25a)

s.t. 
$$\mathbf{\dot{x}}^{[k]}(t) = \mathbf{\hat{f}}\left(\mathbf{x}^{[k]}(t), \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, t\right), \qquad k = 0, \dots, s,$$
 (25b)

$$\boldsymbol{\varphi}(\mathbf{x}^{[0]}(t_0), \mathbf{x}^{[s]}(t_f), t_f) = \mathbf{0}, \tag{25c}$$

$$\mathbf{x}^{[k]}(t_{k+1}) = \mathbf{x}^{[k+1]}(t_{k+1}), \qquad k = 0, \dots, s - 1,$$
(25d)

$$\mathbf{u}^{\min} \leq \boldsymbol{\mu}_1^{[k]} \circ \mathbf{u}^{\min} + \boldsymbol{\mu}_2^{[k]} \circ \mathbf{u}^{\max} + \left(\mathbf{1} - \boldsymbol{\mu}_1^{[k]} - \boldsymbol{\mu}_2^{[k]}\right) \circ \mathbf{u}^{\operatorname{sing}}(t; \mathbf{x}^{[k]}) \leq \mathbf{u}^{\max},$$
  
$$k = 0, \dots, s, \qquad (25e)$$

$$\mu_1^{[k]} + \mu_2^{[k]} \le \mathbf{1}, \qquad k = 0, \dots, s,$$
(25f)

$$\boldsymbol{\mu}_{1}^{[k]}, \ \boldsymbol{\mu}_{2}^{[k]} \in \{0,1\}^{q}, \qquad k = 0, \dots, s,$$
(25g)

such that

$$\begin{split} \mathbf{\hat{f}}\left(\mathbf{x}^{[k]}(t), \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, t\right) = \\ \mathbf{f}\left(\mathbf{x}^{[k]}(t), \boldsymbol{\mu}_{1}^{[k]} \circ \mathbf{u}^{\min} + \boldsymbol{\mu}_{2}^{[k]} \circ \mathbf{u}^{\max} + \left(\mathbf{1} - \boldsymbol{\mu}_{1}^{[k]} - \boldsymbol{\mu}_{2}^{[k]}\right) \circ \mathbf{u}^{\operatorname{sing}}(t; \mathbf{x}^{[k]}), t\right). \end{split}$$

### 4.2 Discretization of the Resulted Binary Optimal Control

In this section, the Radau-pseudospectral method is employed to transcribe the binary optimal control problem (25) to an MBNLP problem. In this way, at first, the time-domains  $[t_{k-1}, t_k], k = 0, \ldots, s$  are mapped into [-1, 1] via the following affine transformations:

$$t = \frac{t_{k+1} - t_k}{2}\tau + \frac{t_{k+1} + t_k}{2}, \qquad k = 0, \dots, s.$$
 (26)

Using these mappings and noting that  $\frac{dt}{d\tau} = \frac{t_{k+1}-t_k}{2}$ , the binary optimal control problem (25) is converted to the following minimization problem in the time-domain [-1, 1]:

min 
$$\mathcal{J}\left(\mathbf{x},\boldsymbol{\mu}_{1}^{[k]},\boldsymbol{\mu}_{2}^{[k]},t_{f}\right) := g\left(\mathbf{x}^{[0]}(-1),\mathbf{x}^{[s]}(1),t_{f}\right)$$
 (27a)

$$\dot{\mathbf{x}}^{[k]}(\tau) = \frac{t_{k+1} - t_k}{2} \hat{\mathbf{f}}(\mathbf{x}^{[k]}(\tau), \boldsymbol{\mu}_1^{[k]}(\tau), \boldsymbol{\mu}_2^{[k]}(\tau), \tau), \qquad k = 0, \dots, s,$$
(27b)

$$\boldsymbol{\varphi}(\mathbf{x}^{[0]}(-1), \mathbf{x}^{[s]}(1), t_f) = \mathbf{0}, \tag{27c}$$

$$\mathbf{x}^{[k]}(1) = \mathbf{x}^{[k+1]}(-1)$$
  $k = 0, \dots, s-1$  (27d)

$$\mathbf{u}^{\min} \le \boldsymbol{\mu}_1^{[k]} \circ \mathbf{u}^{\min} + \boldsymbol{\mu}_2^{[k]} \circ \mathbf{u}^{\max} + \left(\mathbf{1} - \boldsymbol{\mu}_1^{[k]} - \boldsymbol{\mu}_2^{[k]}\right) \circ \mathbf{u}^{\operatorname{sing}}(t; \mathbf{x}^{[k]}) \le \mathbf{u}^{\max},$$
  
$$k = 0, \dots, s, \qquad (27e)$$

$$\boldsymbol{\mu}_{1}^{[k]} + \boldsymbol{\mu}_{2}^{[k]} \le \mathbf{1}, \qquad k = 0, \dots, s,$$
(27f)

$$\boldsymbol{\mu}_{1}^{[k]}, \ \boldsymbol{\mu}_{2}^{[k]} \in \{0,1\}^{q}, \qquad k = 0, \dots, s.$$
 (27g)

It is noted that, by applying this transformation, the symbols of variables will change and new symbols should be used for them. For simplicity, however, we retained the symbols already used.

Now, by considering (16), the *l*-th component of state  $\mathbf{x}^{[k]}(t)$  is approximated by Lagrange polynomials as:

$$x_l^{[k]}(\tau) \simeq \sum_{i=0}^n x_l^{[k]}(\xi_i)\ell_i(\tau), \qquad k = 0, \dots, s.$$
 (28)

So, the vector function  $\mathbf{x}^{[k]}(t)$  is approximated as:

$$\mathbf{x}^{[k]}(\tau) \simeq \sum_{i=0}^{n} \boldsymbol{\alpha}_{i}^{k} \ell_{i}(\tau), \qquad k = 0, \dots, s,$$
(29)

where for  $k = 0, \ldots, s$  and  $i = 0, \ldots, n$ , the coefficients  $\boldsymbol{\alpha}_i^k$  are unknown *p*-vector and

$$\boldsymbol{\alpha}_{i}^{k} = \mathbf{x}^{[k]}(\xi_{i}) = [x_{1}^{[k]}(\xi_{i}), \dots, x_{p}^{[k]}(\xi_{i})]^{T}.$$

Using (29), we have:

$$\dot{\mathbf{x}}^{[k]}(\tau) \simeq \sum_{i=0}^{n} \boldsymbol{\alpha}_{i}^{k} \dot{\ell}_{i}(\tau), \qquad k = 0, \dots, s.$$
(30)

By substituting approximations (29) and (30) in the dynamic equations (27b) and then by collocating it at LGR points  $\xi_j$ , j = 0, ..., n - 1, we get:

$$\sum_{i=0}^{n} \boldsymbol{\alpha}_{i}^{k} \dot{\ell}_{i}(\xi_{j}) - \frac{t_{k+1} - t_{k}}{2} \mathbf{\hat{f}} \left( \sum_{i=0}^{n} \boldsymbol{\alpha}_{i}^{k} \ell_{i}(\xi_{j}), \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, \xi_{j} \right) = 0,$$
  
$$k = 0, \dots, s, \ j = 0, \dots, n-1.$$

It is worthwhile to note that, although  $\xi_n = +1$  is used beside the LGR points to approximate  $\mathbf{x}^{[k]}(\tau)$ , this point is not used as a collocation point.

By (18) and the Kronecker property (17), the above equation is reduced to the following algebraic equations:

$$\sum_{i=0}^{n} \boldsymbol{\alpha}_{i}^{k} d_{ji} = \frac{t_{k+1} - t_{k}}{2} \hat{\mathbf{f}} \left( \boldsymbol{\alpha}_{j}^{k}, \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, \xi_{j} \right), \quad j = 0, ..., n-1, \quad k = 0, \dots, s.$$
(31)

By noting that, for k = 0, ..., s,  $\mathbf{x}^{[k]}(-1) = \boldsymbol{\alpha}_0^{[k]}$  and  $\mathbf{x}^{[k]}(1) = \boldsymbol{\alpha}_n^{[k]}$ , finally, the binary optimal control problem (27) is converted to the following finite-dimensional MBNLP

min 
$$\mathcal{J}\left(\mathbf{x}, \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, t_{f}\right) := g\left(\boldsymbol{\alpha}_{0}^{0}, \boldsymbol{\alpha}_{n}^{s}, t_{f}\right)$$
 (32a)

$$\sum_{i=0}^{n} d_{ji} \boldsymbol{\alpha}_{i}^{k} - \frac{t_{k+1} - t_{k}}{2} \hat{\mathbf{f}} \left( \boldsymbol{\alpha}_{j}^{k}, \boldsymbol{\mu}_{1}^{[k]}, \boldsymbol{\mu}_{2}^{[k]}, \xi_{j} \right) = 0,$$
(32b)

$$j = 0, 1, ..., n - 1, \quad k = 0, ..., s,$$
 (32c)

$$\varphi(\boldsymbol{\alpha}_{0}^{\circ},\boldsymbol{\alpha}_{n}^{\circ},t_{f}) = \mathbf{0}, \tag{32d}$$

$$\boldsymbol{\alpha}^{k} = \boldsymbol{\alpha}^{k+1}_{c} \qquad k = 1 \qquad s-1 \tag{32e}$$

$$\mathbf{u}^{\min} \le \boldsymbol{\mu}_{1}^{[k]} \circ \mathbf{u}^{\min} + \boldsymbol{\mu}_{2}^{[k]} \circ \mathbf{u}^{\max} + \left(\mathbf{1} - \boldsymbol{\mu}_{1}^{[k]} - \boldsymbol{\mu}_{2}^{[k]}\right) \circ \mathbf{u}^{\operatorname{sing}}(t; \mathbf{x}^{[k]}) \le \mathbf{u}^{\max},$$
(22f)

$$k = 0, \dots, s, \tag{32f}$$

$$\mu_1^{[k]} + \mu_2^{[k]} \le \mathbf{1}, \qquad k = 0, \dots, s, \tag{32g}$$

$$\boldsymbol{\mu}_{1}^{[k]}, \ \boldsymbol{\mu}_{2}^{[k]} \in \{0,1\}^{q}, \qquad k = 0, \dots, s.$$
 (32h)

Recall that, the decision variables of the above BINLP are  $\alpha_i^k$ ,  $t_k$ ,  $\mu_1^{[k]}$ ,  $\mu_2^{[k]}$  and maybe  $t_f$ , where  $i = 0, \ldots, n, \ k = 0, \ldots, s$ .

#### 4.3 Selecting the number of initial switching points in the proposed algorithm

As mentioned, in the proposed method, a guess on the number of switching points is needed. In the following, we describe how to choose the number of switching points and how to avoid incorrect choices of s.

Let s be our guess on the number of switching points and  $s^*$  be the exact number of switching points. Based on the choice of s, the following three cases are distinguished:

- I. If  $s = s^*$ , then the proposed method performs best and the approximate position of *i*-th switch is obtained as  $t_i$ .
- II. If  $s < s^*$ , naturally the proposed method cannot find the optimal solution. With this choice, two things happen. Whether MBNLP solver cannot find any feasible solution or the solver converges to a solution that is not optimal.
- III. If  $s > s^*$ , then the proposed method considers  $t_1, \ldots, t_s$  as the candidates of switching points. Naturally, the obtained control function does not switch at any  $t_i$ . Indeed  $s-s^*$  of the obtained  $t_1, \ldots, t_s$  are not switching point and we call them by *artificial switching points*. For instance, when all the components of control function do not change at  $t_i$ , then we can easily recognize that  $t_i$  is not a switching point and we consider it as an artificial switching point. As another instance, if the computation shows that  $t_{i-1} = t_i$ , then  $t_i$  is an artificial switching point too. Moreover, when  $t_i$  and  $t_{i+1}$  are distinct but the difference  $t_{i+1} - t_i$  is very small, then we must consider  $t_i$  and  $t_{i+1}$  as artificial switching points and eliminate the arc between  $t_i$  and  $t_{i+1}$ . This small arc happens because of round-off error in MBNLP solver, however, the length of

this arc is smaller than the considered error tolerance in the used MBNLP solver. It is noted that the artificial switching points do not influence the structure of optimal control.

Based on the above discussions, to capture the exact number of switching points, we apply the proposed method with a guess s. If a solution with some artificial switching points is obtained, then by removing the artificial switching points, the exact number of switching points and structure of optimal control are detected. Otherwise, if either the MBNLP solver fails or a solution without artificial arc is obtained, then, we must try the method with a larger guess for s.

## 5. Illustrative examples

This section is devoted to illustrating the presented method in Section 4, using numerical experiments. We have implemented the method using MATLAB in a personal computer and to solve the final BINLP (32), the solver KNITRO (Byrd, Nocedal, & Waltz, 2006) has been interfaced and function knitromatlab\_mip is used.

We test the feasibility and validity of the presented method on four optimal control problems. Each of these problems highlights one capability of the presented method. In the first, the ability of the presented method in finding the structure of optimal control is illustrated and it is shown that the presented method can be used for solving bang-bang problems as well. In the second example, we show the accuracy of the presented method on the benchmark Goddard's problem. In the third, the ability of the method in solving problems with vector value control is investigated. By the last example, we show that the presented method is applicable to the singular problems with entirely singular control.

### 5.1 Example 1 (Rayleigh Control Problem With Mixed Control-State Constrains)

In this example, we consider the following Rayleigh control problem with mixed control-state constraints (J. Chen & Gerdts, 2012; Maurer & Augustin, 2001; Maurer & Osmolovskii, 2013; Osmolovskii & Maurer, 2012)

$$\begin{array}{ll} \min & \mathcal{J} = x_3(t_f), \\ & \dot{x}_1 = x_2, \\ & \dot{x}_2 = -x_1 + x_2(1.4 - 0.14x_2^2) + u, \\ & \dot{x}_3 = (x_1^2 + x_2^2), \\ & x_1(0) = -5, \quad x_2(0) = -5, \quad x_3(0) = 0, \\ & \alpha \le u(t) + x_1(t) \le \beta, \quad \forall t \in [0, t_f], \end{array}$$

where the final time  $t_f$  is fixed and equal to 4.5. Following Maurer and Osmolovskii (2013), by introducing the new control variable  $v(t) = u(t) + x_1(t)$ , the above Rayleigh problem is transformed to the following problem with box constraints on control v(t)

$$\begin{array}{ll} \min & \mathcal{J} = x_3(t_f), \\ & \dot{x}_1 = x_2, \\ & \dot{x}_2 = -x_1 + x_2(1.4 - 0.14x_2^2) + v - x_1, \\ & \dot{x}_3 = x_1^2 + x_2^2, \\ & x_1(0) = -5, \quad x_2(0) = -5, \quad x_3(0) = 0, \\ & \alpha \le v(t) \le \beta, \quad \forall t \in [0, t_f]. \end{array}$$

The Hamiltonian function of the above optimal control problem is:

$$\mathscr{H}(\mathbf{x}, u, \boldsymbol{\lambda}, t) = \lambda_1 x_2 + \lambda_2 (-x_1 + x_2(1.4 - 0.14x_2^2) + v - x_1) + \lambda_3 (x_1^2 + x_2^2).$$

In this problem the adjoint equations are:

$$\dot{\lambda}_1 = -2x_1 + \lambda_2,\tag{33}$$

$$\dot{\lambda}_2 = -2x_2 - \lambda_1 + \lambda_2(0.42x_2^2 - 1.4), \tag{34}$$

$$\dot{\lambda}_3 = 0. \tag{35}$$

The switching function for v is  $\sigma(\mathbf{x}, \boldsymbol{\lambda}, t) = \lambda_2(t)$ . From the Pontryagin's minimum principle, we conclude

$$v(t) = \begin{cases} \alpha, & \text{if } \lambda_2 > 0, \\ v^{\text{sing}}(x(t)), & \text{if } \lambda_2 = 0, \\ \beta, & \text{if } \lambda_2 < 0. \end{cases}$$

Computing the first two derivatives of the switching function, we get

$$\begin{aligned} \frac{d}{dt}\sigma(\mathbf{x}, \boldsymbol{\lambda}, t) &= \dot{\lambda}_2(t) = -\lambda_1(t) - 2x_2(t), \\ \frac{d^2}{dt^2}\sigma(\mathbf{x}, \boldsymbol{\lambda}, t) &= -\dot{\lambda}_1(t) - 2\dot{x}_2(t), \\ &= 6x_1(t) - 2x_2(t)(1.4 - 0.14x_2^2(t)) - 2v(t). \end{aligned}$$

It can be seen that the control v appears in the second derivative of  $\sigma$ , therefore the order of the problem is  $\kappa = 1$ . Moreover, by extracting v from  $\frac{d^2}{dt^2}\sigma = 0$ , the control function on the singular interval  $[t_1, t_2]$  is obtained as:

$$v = v^{\text{sing}}(\mathbf{x}) = 3x_1 + x_2(0.14x_2^2 - 1.4).$$

Following Maurer and Osmolovskii (2013), we consider three cases for  $\alpha$  and  $\beta$  as:

Case I:  $\alpha = -5, \beta = 0.$ 

Case II:  $\alpha = -8, \beta = 0.$ 

Case III:  $\alpha = -10, \beta = 0.$ 

According to Maurer and Osmolovskii (2013), the structure of optimal control is bang-bang in Case I, bang-bang in Case II and bang-bang-singular in Case III. Accordingly, this example is suitable to test the ability of our method in finding the structure of the optimal control.

Results For Case  $I(\alpha = -5, \beta = 0)$ 

At first, we applied the presented method, with s = 6 and n = 20. The resulted switching points and the control function are obtained as

$$v(t) = \begin{cases} 0, & \text{if} & 0.0 \le t \le 0.779970995585, \\ -5, & \text{if} & 0.779970995585 \le t \le 2.307546460159, \\ 0, & \text{if} & 2.307546460159 \le t \le 2.307546460255, \\ 0, & \text{if} & 2.307546460255 \le t \le 2.307546460351, \\ -5, & \text{if} & 2.307546460351 \le t \le 2.683557086284, \\ 0, & \text{if} & 2.683557086284 \le t \le 4.5. \end{cases}$$

For better vision, the obtaining control is plotted in Figure 1. As we see,  $t_2 = 2.307546460159$ ,  $t_3 = 2.307546460255$  and  $t_4 = 2.307546460351$  are reported as switching points, but these points are very close to each other. As mentioned in Section 4.3, these small differences occur because of error tolerance in MBNLP solver. Inspecting Figure 1, we deduce that these points( $t_2$ ,  $t_3$  and  $t_4$ ) are artificial switching points and can be removed. Accordingly, the exact number of switching points is s = 2.

Next, we apply the presented method with s = 2 and n = 20. In Figure 2, the optimal control and state functions are plotted. To show the accuracy and convergence of the method, the switching points and objective function are reported in Table 1 for various values of n.

It is worth noting that, in Case I, the optimal control is purely bang-bang and not singular. Although the present method is developed for solving SOCPs, it can be applied to the bang-bang problems as well. In other words, in the presented method, we do not need to know that the optimal control is bang-bang or singular.

# Results For Case $II(\alpha = -8, \beta = 0)$

For detecting the structure of optimal control, we first applied the method, with s = 5 and n = 20. The obtained control and state functions are plotted in Figure 3. Clearly, the exact number of switching points is s = 2. To address the accuracy and convergence of the method, in Table 2, the obtained switching points and objective function are reported for various values on n.

## Results For Case III( $\alpha = -10, \beta = 0$ )

At first, in a similar manner to Cases I and II, we found that the exact number of switching points is s = 1.

The obtained control and state functions with n = 20 are plotted in Figure 4. Moreover, the obtained switching points and objective function value are reported in Table 3 for various values on n.

### 5.2 Example 2 (Goddard's Problem)

In the second example, we consider Goddard's problem as presented in Bryson and Ho (1975). This problem now is considered as a benchmark problem for SOCPs (Aronna et al., 2013; Betts, 2010; Bonnans et al., 2008; Martinon, Bonnans, Laurent-Varin, & Trélat, 2009; Maurer, 1976; Vossen, 2010). Goddard's problem is to maximize the final altitude of a vertically ascending rocket under the influence of atmospheric drag and the gravitational field.

This problem is modeled as follows

$$\begin{array}{ll} \max & \mathcal{J} = h(t_f), \\ & \dot{h} = v, \\ & \dot{v} = \frac{1}{m}(cu - D(v,h)) - g(h), \\ & \dot{m} = -u, \\ & h(0) = 0, \quad v(0) = 0, \quad m(0) = m_0, \quad m(t_f) = m_f, \\ & 0 \le u(t) \le u^{\max}, \quad \forall t \in [0, t_f], \end{array}$$

where the final time is free and the state variables are altitude h, speed v and mass m of the rocket during the flight. The control u is the thrust of the rocket. Moreover, D(v, h) and g(h) are the drag

and gravity functions defined as:

$$D(v,h) = \alpha v^2 \exp(-\beta h), \qquad g(h) = g_0.$$

We consider the following two cases for the parameters of the problem

• Case I:

$$\begin{array}{ll} \alpha = 0.01227, & \beta = 0.000145, & g_0 = 9.81, & c = 2060, \\ m_0 = 214.839, & m_f = 67.9833, & u^{\max} = 9.52551. \end{array}$$

• Case II.

$$\alpha = 5.49153485e-5, \quad \beta = 1/23800, \quad g_0 = 32.174, \quad c = 1580.9425, \\ m_0 = 3, \quad m_f = 1, \quad u^{\max} = 193/c.$$

The problem data in Case I and II are taken from Maurer (1976) and Betts (2010), respectively.

According to Aronna et al. (2013); Maurer (1976); Vossen (2010), the problem order is equal to  $\kappa = 1$  and the singular control is obtained as:

$$u^{\rm sing}(h,v,m) = \frac{D}{c} + m \frac{(c-v)D_h + (D_v + cD_{vv})g + c(mg_h - D_{vh}v)}{D + 2cD_v + c^2 D_{vv}}.$$

After applying the present method with s = 4 and n = 20, the resulting control functions in Case I and II are plotted in Fig 5. As a result, we conclude that in the both cases, the structure of optimal control is max-singular-min, i.e. s = 2. To check the accuracy and convergence of the method, in Table 4, the obtained switching points and the objective function with s = 2 are reported for various values on n. The resulting control and state functions, in Case I, with s = 2 and n = 20, are shown in Figure 6.

# 5.3 Example 3 (Mathematical Model For Combined Anti-angiogenesis And Chemotherapy Treatments )

Now, we consider the following tumor anti-angiogenesis and chemotherapy optimal control problem treated in Ledzewicz, Maurer, and Schättler (2009)

$$\begin{array}{ll} \min & \mathcal{J} = p(t_f), \\ & \dot{p} = -\zeta p \ln(\frac{p}{q}) - \varphi p v, \\ & \dot{q} = bq^{\frac{2}{3}} - dq^{\frac{4}{3}} - \mu q - \gamma q u - \eta q v, \\ & \dot{y} = u, \\ & \dot{z} = v, \\ & p(0) = p_0, \quad q(0) = q_0, \quad y(0) = 0, \quad z(0) = 0, \\ & 0 \le u(t) \le 15 \quad \forall t \in [0, t_f], \\ & 0 \le v(t) \le 20 \quad \forall t \in [0, t_f], \\ & z(t_f) \le 135, \\ & y(t_f) \le 45. \end{array}$$

In this problem, u and v are control functions. We consider this optimal control problem with the following parameters

$$\begin{aligned} \zeta &= 0.192, \quad b = 5.85, \quad d = 0.00873, \quad \mu = 0.02, \\ \gamma &= 0.15, \quad \eta = 0.025, \quad \varphi = 0.01 \,. \end{aligned}$$

These parameters are based on biologically validated data (Ledzewicz et al., 2009) and taken from Hahnfeldt, Panigrahy, Folkman, and Hlatky (1999). According to Ledzewicz et al. (2009, 2011), the control v is bang-bang and the control u is singular. Furthermore, in the singular interval, we have

$$\gamma u(t) + \eta v = \psi(\sqrt[3]{q(t)}),$$

where

$$\psi(\theta) = \frac{b - d\theta^{\frac{2}{3}}}{\theta^{\frac{1}{3}}} + 3\zeta \frac{b + d\theta^{\frac{2}{3}}}{b - d\theta^{\frac{2}{3}}} - \mu.$$

For our numerical calculations, we take  $p_0 = 9000$  and  $q_0 = 6000$ . Applying our method with s = 5 and n = 20, the following results are obtained for the control functions

$$u(t) = \begin{cases} 15, & \text{if} & 0.0 \le t \le 0.765171962162, \\ 15, & \text{if} & 0.765171962162 \le t \le 0.952984945517, \\ 15, & \text{if} & 0.952984945517 \le t \le 1.063190258452, \\ u^{sin}, & \text{if} & 1.063190258452 \le t \le 2.333116025109, \\ u^{sin}, & \text{if} & 2.333116025109 \le t \le 4.940379282478, \\ 0, & \text{if} & 4.940379282478 \le t \le 7.515171962157. \end{cases}$$

$$v(t) = \begin{cases} 0, & \text{if} & 0.0 \le t \le 0.765171962162, \\ 20, & \text{if} & 0.765171962162 \le t \le 0.952984945517, \\ 20, & \text{if} & 0.952984945517 \le t \le 1.063190258452, \\ 20, & \text{if} & 1.063190258452 \le t \le 2.333116025109, \\ 20, & \text{if} & 2.333116025109 \le t \le 4.940379282478, \\ 20, & \text{if} & 4.940379282478 \le t \le 7.515171962157. \end{cases}$$

These control functions are plotted in Figure 7. From the obtained results, we conclude that the exact number of switching points is s = 3.

Choosing s = 3 and varying n, the obtained values for switching points and objective function are reported in Table 5. In Figure 8, the obtained control and state functions with n = 20 are plotted.

# 5.4 Example 4 (A particle moving under friction)

As the final example, the following problem is considered (Gong, Kang, & Ross, 2006; Ross, 2015)

$$\begin{array}{ll} \min & \mathcal{J} = \int_0^1 x_2 u, \\ & \dot{x_1} = x_2, \\ & \dot{x_2} = -x_2 + u, \\ & -x_2(t) \leq 0, \\ & x_1(0) = 0, \quad x_2(0) = 1, \\ & x_1(1) = 1, \quad x_2(1) = 1, \\ & 0 \leq u(t) \leq 2, \quad \forall t \in [0, 1], \end{array}$$

It can be shown that the singular control can be obtained as:

$$u^{\rm sing}(\mathbf{x},t) = x_2(t),\tag{36}$$

After applying the present method, with s = 5 and n = 20, the resulting control function is obtained as

	$u^{\text{sing}},$	if	$0 \le t \le 0.140649593909000,$
	$u^{\text{sing}},$	if	$0.140649593909000 \le t \le 0.227909561633000,$
$u(t) = \langle$	$u^{\mathrm{sing}},$	if	$0.227909561633000 \le t \le 0.600924779862000,$
. ,	0,	if	$0.600924779862000 \le t \le 0.600924802286000,$
	$u^{\mathrm{sing}},$	if	$0.600924802286000 \le t \le 1.$

Also, for a better observation, the control function is plotted in Figure 9. According to this figure, we find that the control is entirely singular, i.e. s = 0. Now, after detecting the structure of the optimal control problem, the presented method is applied to the problem, with s = 0 and n = 20 and the obtained control and states functions are plotted in Figure 10. As we see, this method can efficiently solve the problems with entirely singular control.

#### 6. Conclusion

The proposed method represented a unified approach for finding the structure of optimal control and accurate solution of SOCPs. The main idea is that by introducing binary variables and utilizing Legendre-Radau pseudospectral method, the singular optimal control problem is transcribed to an MBNLP problem. In addition, the control function is considered as feedback form and the state variable is approximated by a piecewise continuous polynomial. The computational technique was illustrated on four benchmark problems. The results showed that the present method successfully detects the structure of the optimal control function without a priori information and captures switching points with high accuracy, even by using a small number of collocation points.

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Figure 1. (Rayleigh Problem-Case I) The obtained Control function with s = 6 and n = 20.



Figure 2. (Rayleigh Problem-Case I) The obtained state and control functions with s = 2 and n = 20.



Figure 3. (Rayleigh Problem-Case II) The obtained state and control functions with s = 5 and n = 20.



Figure 4. (Rayleigh Problem-Case III) The obtained state and control functions with s = 1 and n = 20.



Figure 5. (Goddard Problem-Cases I and II) The obtained control history with s = 4 and n = 20.



Figure 6. (Goddard Problem-Case I) The obtained state and control functions with s = 2 and n = 20.

Table 1. (Rayleigh Problem-Case I) The obtained values of switching times and performance index for s = 2 and various values of n.

n	$t_1$	$t_2$	${\mathcal J}$
5	<b>0.7</b> 62366612521	<b>2.68</b> 6623895525	<b>62.1</b> 59210594759
10	<b>0.7</b> 80002093663	<b>2.68355</b> 0480205	<b>62.1651</b> 84675530
12	<b>0.779970</b> 073508	<b>2.683557</b> 300887	<b>62.165171</b> 125420
15	<b>0.77997099</b> 4514	<b>2.683557086</b> 664	<b>62.16517137</b> 2819
18	<b>0.77997099</b> 5257	<b>2.683557086</b> 495	<b>62.1651713729</b> 70
20	<b>0.77997099</b> 6007	<b>2.683557086</b> 330	$62.1651713729_{60}$



Figure 7. (Tumor Anti-Angiogenesis and Chemotherapy Problem) The obtained control function with s = 5 and n = 20.



Figure 8. (Tumor Anti-Angiogenesis and Chemotherapy Problem) The obtained state and control functions with s = 3 and n = 20.



Figure 9. (A particle moving under friction) The obtained control function with s = 5 and n = 20.



Figure 10. (A particle moving under friction) The obtained state and control functions with s = 1 and n = 20.

$\overline{n}$	$t_1$	$t_2$	$\mathcal J$
5	<b>0.880</b> 015547157	<b>2.0544</b> 54140463	<b>58.090</b> 656805179
10	<b>0.880</b> 219799773	<b>2.0544</b> 27603716	<b>58.090</b> 500334180
12	<b>0.880194</b> 766862	<b>2.054430</b> 279825	58.090498130729
15	<b>0.8801945</b> 44846	<b>2.054430</b> 308001	<b>58.090498</b> 220480
18	<b>0.88019453</b> 2908	<b>2.054430</b> 291559	<b>58.090498</b> 194399
20	<b>0.88019453</b> 4140	<b>2.054430309</b> 052	<b>58.090498215</b> 789
22	<b>0.88019453</b> 3669	<b>2.054430309</b> 176	<b>58.090498215</b> 940

Table 2. (Rayleigh Problem-Case II) The obtained values of switching times and performance index for s = 2 and various values of n.

Table 3. (Rayleigh Problem-Case III) The obtained values of switching time and performance index for s = 1 and various values of n.

$\overline{n}$	$t_1$	$\mathcal{J}$
5	<b>0.9132</b> 22334416	<b>58.00</b> 0599024549
10	<b>0.91324</b> 7093644	58.001683110229
12	<b>0.9132467</b> 67042	<b>58.00170</b> 760159
15	<b>0.9132467</b> 41986	58.001700222990
18	<b>0.913246741</b> 800	<b>58.001700235</b> 780
20	<b>0.9132467 41 799</b>	<b>58.001700235</b> 910

Table 4. (Goddard Problem) The obtained values of switching times, final time and performance index for various values of n.

Case	n	$t_1$	$t_2$	$t_f$	$\mathcal J$
	5	3.8962984347	<b>46</b> .0628324467	<b>206</b> 4411581494	<b>157</b> 254.0220728
	10	4.1208322283	45.9617898769	<b>206.6</b> 904108521	157346.7714617
	15	4.1209123258	45.9608091368	<b>206.692</b> 7763403	157347.3567926
Case I.	20	4.1209139238	45.9608128828	206.6926967098	157347.3570357
	25	4.1209116491	45.9608174215	206.6928010327	157347.3570367
	30	4.1209116962	45.9608168451	206.6929168216	157347.3570367
	5	13.75358711054	<b>21.98</b> 402662383	<b>42.88</b> 484515140	157254.0220728
	10	13.75524832958	<b>21.988</b> 89104879	<b>42.889</b> 90410852	157346.7714617
Case II.	15	13.75531085002	<b>21.98893</b> 805934	42.8890787640	157347.3567926
	20	13.75531021839	<b>21.98893476</b> 820	42.8890786696	18549.5866295
	25	13.75531021821	<b>21.98893476</b> 769	${\bf 42.88907866} 99$	18549.5866295

Table 5. (Tumor Anti-angiogenesis and Chemotherapy Problem) The obtained values of switching times, final time and performance index for various values of n.

n	$t_1$	$t_2$	$t_3$	$t_f$	${\mathcal J}$
5	<b>0.765</b> 3950	1.0630676	<b>4.940</b> 685	<b>7.515</b> 3950	<b>213.5180</b> 8362
10	<b>0.7654</b> 275	1.0630519	4.9407259	7.5154275	<b>213.5180436</b> 2
12	0.7654079	1.0630615	4.9407013	7.5154079	<b>213.5180436</b> 9
15	0.7654078	1.0630615	4.9407013	7.5154078	213.51804368
18	0.7654078	1.0630615	4.9407013	7.5154078	<b>213.51804368</b>