Proceedings of the 5th International Conference on Optimization and Control with Applications (OCA2012), Beijing, China, December 4-8, 2012

39 A CLASS OF MAX-MIN OPTIMAL CONTROL PROBLEMS WITH APPLICATIONS TO CHROMATOGRAPHY

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Abstract: In this paper, we consider a class of non-standard optimal control problems in which the objective function is in max-min form and the state variables evolve over different time horizons. Such problems arise in the control of gradient elution chromatography—an industrial process used to separate and purify multi-component chemical mixtures. We develop a computational method for solving this class of optimal control problems based on the control parameterization technique, a time-scaling transformation, and a new exact penalty method.

Key words: Optimal control; Control parameterization; Time-scaling transformation; Exact penalty function.

1 PROBLEM STATEMENT

Consider a master system consisting of m coupled subsystems. The dynamics of the ith subsystem are described by the following set of ordinary differential equations:

$$\dot{\boldsymbol{x}}^i(t) = \boldsymbol{f}^i(\boldsymbol{x}^1(t), \ldots, \boldsymbol{x}^m(t), \boldsymbol{u}(t))\chi_{[0,\tau_i]}(t), \quad t \geq 0, \tag{1.1}$$

$$\boldsymbol{x}^i(0) = \boldsymbol{\zeta}^i, \tag{1.2}$$

where $\boldsymbol{x}^i(t) \in \mathbb{R}^n$ is the *state* of the ith subsystem, τ_i is the *terminal time* of the ith subsystem (a free decision variable), $\boldsymbol{\zeta}^i \in \mathbb{R}^n$ is the initial state of the ith subsystem (a given vector), $\boldsymbol{u}(t) \in \mathbb{R}^r$ is the *control input*, and the indicator function $\chi_{[0,\tau_i]} : \mathbb{R} \to \mathbb{R}$ is defined by

$$\chi_{[0,\tau_i]}(t) = \begin{cases} 1, & \text{if } t \in [0, \tau_i], \\ 0, & \text{if } t \notin [0, \tau_i]. \end{cases}$$

We assume that $\boldsymbol{f}^i : \mathbb{R}^{mn} \times \mathbb{R}^r \to \mathbb{R}^n$ in (1.1) is a given continuously differentiable function.

The control function in (1.1) is subject to the following bound constraints:

$$a_j \leq u_j(t) \leq b_j, \quad t \geq 0, \quad j = 1, \ldots, r, \tag{1.3}$$

where $u_j(t)$ is the jth element of $\boldsymbol{u}(t)$ and a_j and b_j are given constants such that $a_j < b_j$. Any measurable function $\boldsymbol{u} : [0, \infty) \to \mathbb{R}^r$ satisfying (1.6) is called an *admissible control*. Let $\mathcal{U}$ denote the class of all such admissible controls.

We collect the subsystem terminal times into a vector $\boldsymbol{\tau} = [\tau_1, \ldots, \tau_m] \in \mathbb{R}^m$. Let $\mathcal{T}$ denote the set of all such vectors with components satisfying $\tau_i \geq 0$, $i = 1, \ldots, m$. Furthermore, let T denote the terminal time of the overall system. Then clearly,

$$T = \max\{\tau_1, \ldots, \tau_m\}.$$

The subsystems described by (1.1)-(1.2) are subject to the following *terminal state constraints*:

$$\Phi_i(\boldsymbol{x}^i(\tau_i)) = 0, \quad i = 1, \ldots, m, \tag{1.4}$$

where each $\Phi_i : \mathbb{R}^n \to \mathbb{R}$ is a given continuously differentiable function.

Our optimal control problem is stated below.

Problem 1 Choose $\boldsymbol{\tau} \in \mathcal{T}$ and $\boldsymbol{u} \in \mathcal{U}$ to maximize the objective functional

$$J(\boldsymbol{\tau}, \boldsymbol{u}) = \min_{i \neq j} \Psi(\tau_i, \tau_j, T, \boldsymbol{x}^i(\tau_i), \boldsymbol{x}^j(\tau_j)), \tag{1.5}$$

subject to the dynamic system (1.1)-(1.2) and the constraints (1.4), where $\Psi : \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a given continuously differentiable function.

Problem 1 presents two major challenges for existing optimal control methods: (i) the objective functional is non-smooth; and (ii) the state variables are defined over different time horizons.

Farhadinia et al. (see Farhadinia B. (2009)) developed a computational method for solving Problem 1 with $\Psi = -T$. In this case, Problem 1 reduces to a time-optimal control problem in which the aim is to minimize the terminal time of the overall system. Our goal in this paper is to develop a new method that is applicable to more general problems.

2 APPLICATIONS TO CHROMATOGRAPHY

Optimal control problems in the form of Problem 1 arise in chromatography—a separation and purification process that plays an important role in many industrial settings. A typical chromatography system consists of a column containing an absorbent (called the stationary phase) and a liquid that flows through the column (called the mobile phase). The mixture to be separated is injected into the mobile phase and flows through the column. Because the different components in the mixture are attracted to the stationary phase in different degrees, they travel through the column at different speeds, and thus they exit the column at different times (called retention times). Therefore, the mixture is gradually separated while moving through the column.

Jennings et al. (Jennings L. S. (1995)) and Chai et al. (Chai Q. (2012)) have considered a special case of Problem 1 in which the aim is to maximize separation efficiency in a chromatography system. In this problem, the subsystems correspond to the different components in the mixture, and the terminal times are the retention times. The terminal state constraints (1.4) arise because of a requirement that the concentration of each component reach a given value at the corresponding retention time. Meanwhile, the objective functional, which is obtained by setting $\Psi = (\tau_j - \tau_i)^2/T$ in equation (1.5), measures the minimum duration between successive retention times—a quantity that should be maximized.

3 CONTROL PARAMETERIZATION

In this section, we apply the control parameterization method (see Teo K. L. (1991)) to approximate Problem 1 by a finite-dimensional optimization problem.

Let $p \geq 1$ be a given integer. We approximate the control $\boldsymbol{u}$ in (1.1)-(1.2) by a piecewise-constant function that switches value at each terminal time and at $p-1$ locations between each pair of consecutive terminal times. The approximate control is defined as follows:

$$\boldsymbol{u}^p(t) = \sum_{k=1}^{mp} \boldsymbol{\sigma}^k \chi_{[t_{k-1}, t_k)}(t), \tag{3.1}$$

where t_k is the kth control switching time, $\boldsymbol{\sigma}^k \in \mathbb{R}^r$ is the control value on subinterval $[t_{k-1}, t_k)$, and the characteristic function $\chi_{[t_{k-1}, t_k)} : \mathbb{R} \to \mathbb{R}$ is as defined in Section 1. The control switching times satisfy

$$0 = t_0 \leq t_1 \leq t_2 \leq \cdots \leq t_{mp-1} \leq t_{mp} = T. \tag{3.2}$$

Furthermore, every pth control switching time coincides with one of the subsystem terminal times.

In view of (1.6), we have the following constraints on the control values:

$$a_j \leq \sigma_j^k \leq b_j, \quad j = 1, \ldots, r, \quad k = 1, \ldots, mp, \tag{3.3}$$

where σ_j^k is the jth component of $\boldsymbol{\sigma}^k$.

Let

$$v_{ij} = \begin{cases} 1, & \text{if subsystem } i \text{ has the } j\text{th earliest terminal time,} \\ 0, & \text{otherwise.} \end{cases}$$

Hence, if $v_{ij} = 1$, then subsystem i terminates at time $t = t_{jp}$. Clearly,

$$\sum_{j=1}^{m} v_{ij} = 1, \quad i = 1, \ldots, m, \tag{3.4}$$

and

$$\sum_{i=1}^{m} v_{ij} = 1, \quad j = 1, \ldots, m. \tag{3.5}$$

Substituting the approximate control defined by (3.1) into the dynamic system (1.1)-(1.2) yields

$$\dot{\boldsymbol{x}}^i(t) = \sum_{j=1}^{m} v_{ij} \boldsymbol{f}^i(\boldsymbol{x}^1(t), \ldots, \boldsymbol{x}^m(t), \boldsymbol{\sigma}^k) \chi_{[0,t_{jp}]}(t), \quad t \in [t_{k-1}, t_k), \quad k = 1, \ldots, mp, \tag{3.6}$$

$$\boldsymbol{x}^i(0) = \boldsymbol{\zeta}^i. \tag{3.7}$$

Furthermore, the terminal constraints (1.4) become

$$\sum_{j=1}^{m} v_{ij} \Phi(\boldsymbol{x}^i(t_{jp})) = 0, \quad i = 1, \ldots, m. \tag{3.8}$$

The binary constraints $v_{ij} \in \{0, 1\}$ are difficult to enforce explicitly. Hence, we replace $v_{ij} \in \{0, 1\}$ with the following set of *non-discrete* constraints:

$$\sum_{j=1}^{m} v_{ij}(j^2 - j + \tfrac{1}{3}) - \left\{ \sum_{j=1}^{m} v_{ij}(j - \tfrac{1}{2}) \right\}^2 = \frac{1}{12}, \quad i = 1, \ldots, m, \tag{3.9}$$

and

$$0 \leq v_{ij} \leq 1, \quad i = 1, \ldots, m, \quad j = 1, \ldots, m. \tag{3.10}$$

The following theorem, proved in Chai et al. (Chai Q. (2012)), shows that (3.9) and (3.10) imply $v_{ij} \in \{0, 1\}$.

Theorem 3.1 *Suppose that* v_{ij}, $i = 1, \ldots, m$, $j = 1, \ldots, m$ *satisfy* (3.4) *and* (3.10). *Then for each* $i = 1, \ldots, m$, *equation* (3.9) *holds if and only if there exists a* $q \in \{1, \ldots, m\}$ *such that* $v_{iq} = 1$ *and* $v_{ij} = 0$ *for all* $j \neq q$.

The subsystem terminal times occur at $t = t_{jp}$, $j = 1, \ldots, m$. Let q_j denote the unique index satisfying $v_{q_j j} = 1$. Then

$$\boldsymbol{x}^{q_j}(t_{jp}) = v_{1j} \boldsymbol{x}^1(t_{jp}) + \cdots + v_{mj} \boldsymbol{x}^m(t_{jp}). \tag{3.11}$$

We can now state the following finite-dimensional approximation of Problem 1.

Problem 2 Choose t_k and $\boldsymbol{\sigma}^k$, $k = 1, \ldots, mp$ and v_{ij}, $i = 1, \ldots, m$, $j = 1, \ldots, m$ to maximize the objective function

$$J^p = \min_{i \neq j} \Psi(t_{ip}, t_{jp}, t_{mp}, \boldsymbol{x}^{q_i}(t_{ip}), \boldsymbol{x}^{q_j}(t_{jp}))$$

subject to the dynamic system (1.7)-(3.7) and the constraints (3.2)-(3.5) and (3.8)-(3.10).

4 TIME-SCALING TRANSFORMATION

Standard optimization algorithms will struggle with Problem 2 because the switching times in (1.7)-(3.7) are variable (see Loxton R. (2008)). Thus, in this section, we will apply a novel time-scaling transformation to map the switching times to fixed points in a new time horizon. To do this, we introduce a new time variable $s \in [0, mp]$ and relate s to t through the following differential equation:

$$\frac{dt(s)}{ds} = \omega(s), \quad t(0) = 0, \tag{4.1}$$

where $\omega : [0, mp] \to [0, \infty)$ is a piecewise-constant function with fixed switching times at $s = 1, \ldots, mp-1$. We express ω mathematically as follows:

$$\omega(s) = \sum_{k=1}^{mp} \theta_k \chi_{[k-1,k)}(s),$$

where $\theta_k = t_k - t_{k-1}$ is the duration between consecutive switching times in the original time horizon. Clearly,

$$\theta_k \geq 0, \quad k = 1, \ldots, mp. \tag{4.2}$$

For $s \in [k-1, k]$, integrating (4.1) gives

$$t(s) = \int_0^s \omega(\eta) d\eta = \sum_{l=1}^{k-1} \theta_l + \theta_k (s - k + 1).$$

Thus, for each $k = 1, \ldots, mp$,

$$t(k) = \sum_{l=1}^{k} \theta_l = \sum_{l=1}^{k} (t_l - t_{l-1}) = t_k.$$

This shows that the time-scaling transformation defined by (4.1) maps $t = t_k$ to the fixed integer $s = k$. In particular, the terminal time $t = T$ is mapped to $s = mp$:

$$t(mp) = \sum_{k=1}^{mp} \theta_k = t_{mp} = T = \max\{\tau_1, \ldots, \tau_m\}.$$

After applying the time-scaling transformation, the approximate control (3.1) becomes

$$\tilde{\boldsymbol{u}}^p(s) = \boldsymbol{u}^p(t(s)) = \sum_{k=1}^{mp} \boldsymbol{\sigma}^k \chi_{[k-1,k)}(s).$$

Furthermore, the dynamic system (1.7)-(3.7) becomes

$$\dot{\tilde{\boldsymbol{x}}}^i(s) = \sum_{j=1}^{m} v_{ij} \theta_k \boldsymbol{f}^i(\tilde{\boldsymbol{x}}^1(s), \ldots, \tilde{\boldsymbol{x}}^m(s), \boldsymbol{\sigma}^k) \chi_{[0,jp]}(s), \quad s \in [k-1, k), \quad k = 1, \ldots, mp, \tag{4.3}$$

$$\tilde{\boldsymbol{x}}^i(0) = \boldsymbol{\zeta}^i, \tag{4.4}$$

where $\tilde{\boldsymbol{x}}^i(s) = \boldsymbol{x}^i(t(s))$. Constraints (3.8) become

$$\sum_{j=1}^{m} v_{ij} \Phi(\tilde{\boldsymbol{x}}^i(jp)) = 0, \quad i = 1, \ldots, m. \tag{4.5}$$

Also, (3.11) becomes

$$\tilde{\boldsymbol{x}}^{q_j}(jp) = v_{1j} \tilde{\boldsymbol{x}}^1(jp) + \cdots + v_{mj} \tilde{\boldsymbol{x}}^m(jp).$$

We now state the following transformed optimal control problem, which is equivalent to Problem 2.

Problem 3 Choose θ_k and $\boldsymbol{\sigma}^k$, $k = 1, \ldots, mp$ and v_{ij}, $i = 1, \ldots, m$, $j = 1, \ldots, m$ to maximize the objective function

$$\tilde{J}^p = \min_{i \neq j} \tilde{\Psi}(\boldsymbol{\theta}, \tilde{\boldsymbol{x}}^{q_i}(ip), \tilde{\boldsymbol{x}}^{q_j}(jp))$$

subject to the dynamic system (4.3)-(4.4) and the constraints (3.3)-(3.5), (3.9), (3.10), (4.2), and (4.5), where

$$\tilde{\Psi}(\boldsymbol{\theta}, \tilde{\boldsymbol{x}}^{q_i}(ip), \tilde{\boldsymbol{x}}^{q_j}(jp)) = \Psi(\theta_1 + \cdots + \theta_{ip}, \theta_1 + \cdots + \theta_{jp}, \theta_1 + \cdots + \theta_{mp}, \tilde{\boldsymbol{x}}^{q_i}(ip), \tilde{\boldsymbol{x}}^{q_j}(jp)).$$

5 TRANSFORMATION INTO SMOOTH FORM

In this section, we transform Problem 3 into a smooth optimization problem. Let ξ be a new decision variable, where

$$\xi = \min_{i \neq j} \tilde{\Psi}(\boldsymbol{\theta}, \tilde{\boldsymbol{x}}^{q_i}(ip), \tilde{\boldsymbol{x}}^{q_j}(jp)).$$

Then we have the following set of inequality constraints:

$$\tilde{\Psi}(\boldsymbol{\theta}, \tilde{\boldsymbol{x}}^{q_i}(ip), \tilde{\boldsymbol{x}}^{q_j}(jp)) \geq \xi, \quad i \neq j. \tag{5.1}$$

It is clear that Problem 3 is equivalent to the following smooth optimization problem.

Problem 4 Choose ξ, θ_k, $\boldsymbol{\sigma}^k$, and v_{ij} to maximize the objective function $\bar{J}^p(\xi) = \xi$ subject to the dynamic system (4.3)-(4.4) and the constraints (3.3)-(3.5), (3.9), (3.10), (4.2), (4.5), and (5.1).

Standard optimization algorithms will typically struggle with Problem 4 because constraints (3.4), (3.5), (3.9), and (3.10) restrict v_{ij} to be binary decision variables. In the next section, we will describe an exact penalty method for solving Problem 4.

6 AN EXACT PENALTY METHOD

Define

$$\boldsymbol{\gamma} = \left[\xi, \theta_1, \ldots, \theta_{mp}, (\boldsymbol{\sigma}^1)^\top, \ldots, (\boldsymbol{\sigma}^{mp})^\top, (\boldsymbol{v}^1)^\top, \ldots, (\boldsymbol{v}^m)^\top\right]^\top, \tag{6.1}$$

where

$$\boldsymbol{v}^i = [v_{i1}, \ldots, v_{im}]^\top.$$

Furthermore, define a *constraint violation function* as follows:

$$\begin{aligned}\Delta(\boldsymbol{\gamma}) = &\sum_{i=1}^m \left\{ \sum_{j=1}^m v_{ij} - 1 \right\}^2 + \sum_{j=1}^m \left\{ \sum_{i=1}^m v_{ij} - 1 \right\}^2 + \sum_{i=1}^m \left\{ \sum_{j=1}^m v_{ij} \Phi(\tilde{\boldsymbol{x}}^i(jp)) \right\}^2 \\ &+ \sum_{i=1}^m \left\{ \sum_{j=1}^m v_{ij}(j^2 - j + \tfrac{1}{3}) - \left[\sum_{j=1}^m v_{ij}(j - \tfrac{1}{2}) \right]^2 - \tfrac{1}{12} \right\}^2 + \sum_{\substack{i,j=1,\ldots,m \\ i \neq j}} \max\{\xi - \tilde{\Psi}(\boldsymbol{\theta}, \tilde{\boldsymbol{x}}^i(ip), \tilde{\boldsymbol{x}}^j(jp)), 0\}^2,\end{aligned}$$

where $\boldsymbol{\gamma}$ is defined by (6.1). Clearly, $\Delta(\boldsymbol{\gamma}) = 0$ if and only if the current values of the decision variables are feasible for Problem 4.

Define a penalty function as follows:

$$G^p_\mu(\epsilon, \boldsymbol{\gamma}) = -\xi + \epsilon^{-\alpha}\Delta(\boldsymbol{\gamma}) + \mu\epsilon^\beta, \tag{6.2}$$

where ϵ is a new decision variable, $\mu > 0$ is the penalty parameter, and α and β are fixed constants satisfying $1 \leq \beta \leq \alpha$. The new decision variable ϵ is subject to the following bound constraints:

$$0 \leq \epsilon \leq \bar{\epsilon}, \tag{6.3}$$

where $\bar{\epsilon} > 0$ is a given constant.

In the penalty function (6.2), the last term $\mu\epsilon^\beta$ is designed to penalize large values of ϵ, while the middle term $\epsilon^{-\alpha}\Delta(\boldsymbol{\gamma})$ is designed to penalize constraint violations. When μ is large, minimizing (6.2) forces ϵ to be small, which in turn causes $\epsilon^{-\alpha}$ to become large, and thus constraint violations are penalized very severely. Hence, minimizing the penalty function for large values of μ will likely lead to feasible points. On this basis, we can approximate Problem 4 by the following *penalty problem*.

Problem 5 Choose ϵ and $\boldsymbol{\gamma}$ to minimize the penalty function $G^p_\gamma(\epsilon, \boldsymbol{\gamma})$ subject to the dynamic system (4.3)-(4.4) and the bound constraints (3.3), (3.10), (4.2), and (6.3).

Problem 5 can be viewed as an optimal parameter selection problem with multiple characteristic times. Such problems can be solved effectively using the computational method described in Loxton R. (2008), which uses gradient-based optimization techniques. It can be shown that under mild assumptions, when the penalty parameter μ is sufficiently large, any local solution of Problem 5 generates a corresponding local solution for Problem 4 (see Lin Q. (2012)). Thus, the penalty function (6.2) is *exact* in the sense that feasibility is attained for finite values of the penalty parameter.

Solving Problem 2 amounts to solving Problem 5 for an increasing sequence of penalty parameters, where the solution at each iteration is used as the initial guess for the next iteration. The solution of Problem 2 can be used to generate a suboptimal control for Problem 1 through equation (3.1). See Chai Q. (2012) and Lin Q. (2012) for more details.

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