Automatica 95 (2018) 306–315

Contents lists available at ScienceDirect

Automatica

journal homepage: www.elsevier.com/locate/automatica

Free-endpoint optimal control of inhomogeneous bilinear ensemble systems[☆]

Shuo Wang, Jr-Shin Li *

Department of Electrical and Systems Engineering, Washington University in St. Louis, St. Louis, MO, 63130, USA

ARTICLE INFO

Article history:
Received 17 November 2016
Received in revised form 22 January 2018
Accepted 24 April 2018

Keywords:
Ensemble control
Bilinear systems
Iterative method

ABSTRACT

Optimal control of bilinear systems has been a well-studied subject in the areas of mathematical and computational optimal control. However, effective methods for solving emerging optimal control problems involving an ensemble of deterministic or stochastic bilinear systems are underdeveloped. These burgeoning problems arise in diverse applications from quantum control and molecular imaging to neuroscience. In this work, we develop an iterative method to find optimal controls for an inhomogeneous bilinear ensemble system with free-endpoint conditions. The central idea is to represent the bilinear ensemble system at each iteration as a time-varying linear ensemble system, and then solve it in an iterative manner. We analyze convergence of the iterative procedure and discuss optimality of the convergent solutions. The method is directly applicable to solve the same class of optimal control problems involving a stochastic bilinear ensemble system driven by independent additive noise processes. We demonstrate the robustness and applicability of the developed iterative method through practical control designs in neuroscience and quantum control.

1. Introduction

Controlling a population system consisting of a large number of structurally identical dynamic units is an essential step that enables many cutting-edge applications in science and engineering. For example, in quantum science and technology, synchronization engineering, and circadian biology, a central control task is to design exogenous forcing that guides individual subsystems in the population or ensemble to behave in a desired or an optimal manner (Ching & Ritt, 2013; Cory, Fahmy, & Havel, 1997; Kiss, Rusin, Kori, & Hudson, 2007; Ledzewicz & Schättler, 2002; Li & Khaneja, 2006; Pryor, 2006). Such optimal "broadcast" control designs are of theoretical and computational challenge because, in practice, only a single or sparsely distributed control signals are available to engineer individual or collective behavior of many or a continuum of dynamical systems (Li, Dasanayake, & Ruths, 2013; Phelps, Gong, Royset, Walton, & Kaminer, 2014; Ruths & Li, 2012).

There exist numerous numerical methods for solving optimal control problems of nonlinear systems (Rao, 2009), many of which rely heavily on applying effective discretization schemes to discretize the system dynamics and then implementing numerical optimizations to solve the resulting nonlinear programs (NLPs) (Gong, Kang, & Ross, 2006). Canonical methods include direct and indirect shooting methods (Stoer & Bulirsch, 1980; von Stryk & Bulirsch, 1992) and spectral collocation methods such as the pseudospectral method (Gong, Ross, Kang, & Fahroo, 2008). Implementing these commonly-used computational methods to solve optimal control problems involving an ensemble system may encounter low efficiency, slow convergence, and instability issues. It is because each subsystem in the ensemble has an identical structure so that the resulting discretized large-scale NLPs are equipped with a distinctive sparse structure, and, furthermore, each subsystem shares a common control input so that these NLPs involve highly localized and restrictive constraints (Li, Ruths, Yu, Arthanari, & Wagner, 2011).

In this paper, we study the optimal control of a bilinear ensemble system with inhomogeneous natural and translational dynamics, which models a wide range of practical optimal control design problems across disciplines, for example, optimal pulse design in quantum control (Chen, Dong, Long, Petersen, & Rabitz, 2014; Ruths & Li, 2011) and molecular imaging (Woods, Woessner, & Sherry, 2006), motion planning of robots in the presence of uncertainty (Becker & Bretl, 2012), and optimal stimulation of spiking neurons (Ching & Ritt, 2013). In our previous study, we investigated ensemble control designs in these compelling applications and, in particular, focused on devising minimum-energy controls with

☆ This work was supported in part by the NSF awards CMMI-1462796 and ECCS-1509342, the NIH grant 1R21-EY027590-01, and the AFOSR grant FA9550-17-1-0166. The material in this paper was not presented at any conference. This paper was recommended for publication in revised form by Associate Editor James Lam under the direction of Editor Ian R. Petersen.

* Corresponding author.
E-mail addresses: swang35@wustl.edu (S. Wang), jsli@wustl.edu (J.-S. Li).

https://doi.org/10.1016/j.automatica.2018.05.009
0005-1098/© 2018 Elsevier Ltd. All rights reserved.

fixed-endpoint constraints (Wang & Li, 2015). Here, we relax the terminal constraint and study the free-endpoint quadratic optimal bilinear ensemble control problem, where we consider tradeoffs between the terminal cost and control energy. The procedure is based on constructing and solving a corresponding optimal control problem involving a linear ensemble system at each iteration, which is numerically tractable as shown in our previous work (Li, 2011; Zlotnik & Li, 2012). Moreover, the established iterative method is directly applicable to find optimal controls for stochastic bilinear systems driven by additive noise, such as Poisson counters and Brownian motion. We note that iterative methods have been developed for solving free-endpoint optimal control problems (Hofer & Tibken, 1988) or optimal tracking (Çimen & Banks, 2004) of a single deterministic bilinear system. These previous studies lay the foundation of our new developments towards solving optimal control problems involving a bilinear ensemble system governed by inhomogeneous drift and translational dynamics.

This paper is organized as follows. In the next section, formulate the optimal control problem involving a single inhomogeneous bilinear system. We present the iterative method to solve this optimal control problem and show the convergence of the iterative algorithm by using the fixed-point theorem. In Section 3, we extend the iterative method to deal with optimal control problems for bilinear ensemble systems. In Section 4, we illustrate the robustness and applicability of the iterative method through the examples of controlling spiking neurons in the presence of jump processes and pulse design in protein nuclear magnetic resonance (NMR) spectroscopy.

2. Optimal control of inhomogeneous bilinear systems

In this paper, we study optimal control problems involving an ensemble of inhomogeneous bilinear systems with state-invariant drift and translational dynamics of the form

$$\frac{d}{dt}X(t,\beta) = A(\beta)X(t,\beta) + B(\beta)u(t) + \Big[\sum_{i=1}^{m} u_i(t)B_i(\beta)\Big]X(t,\beta) + g(\beta), \tag{1}$$

where $X(t,\beta) \in \mathbb{R}^n$ denotes the state, $\beta \in K \subset \mathbb{R}^d$ is the system parameter varying on the compact set K in the d-dimensional Euclidean space; $u = (u_1, \ldots, u_m)^T$ is the control function with $u_i : [0, t_f] \to \mathbb{R}$ being piecewise continuous; $A \in C(K; \mathbb{R}^{n\times n})$, $B \in C(K; \mathbb{R}^{n\times m})$, and $B_i \in C(K; \mathbb{R}^{n\times n})$, $i = 1, \ldots, m$, are real matrices whose elements are continuous functions over K, and $g \in C(K; \mathbb{R}^n)$. Specifically, we consider the free-endpoint optimal control minimizing the cost functional involving the trade-off between the terminal cost and the energy of the control input.

In the following, we develop an iterative procedure for solving this challenging optimal ensemble control problem. To fix the idea, we first illustrate the framework through a free-endpoint, finite-time, quadratic optimal control problem involving a single deterministic time-invariant inhomogeneous bilinear system. Namely, we consider the problem

$$\begin{aligned} \min \quad & J = \frac{1}{2}\int_0^{t_f} u^T(t)Ru(t)\,dt + \|x(t_f) - x_d\|_2^2, \\ \text{s.t.} \quad & \dot{x} = Ax + Bu + \Big[\sum_{i=1}^{m} u_iB_i\Big]x + g, \end{aligned} \tag{P1}$$

where $x(t) \in \mathbb{R}^n$ is the state and $u(t) = (u_1, \ldots, u_m)^T \in \mathbb{R}^m$ is the control with each u_i piecewise continuous; $A \in \mathbb{R}^{n\times n}$, $B_i \in \mathbb{R}^{n\times n}$, and $B \in \mathbb{R}^{n\times m}$ are constant matrices, and $g \in \mathbb{R}^n$ is a constant vector. In the cost functional, $R \in \mathbb{R}^{m\times m} \succ 0$ is a positive definite weight matrix for the control energy and $\|x(t_f) - x_d\|_2^2 = (x(t_f) - x_d)^T(x(t_f) - x_d)$ represents the terminal cost with respect to the desired state $x_d \in \mathbb{R}^n$. In addition, we can represent the time-invariant bilinear system in (P1) as $\dot{x} = Ax + Bu + \big[\sum_{j=1}^{n} x_j(t)N_j\big]u + g$, in which we write the bilinear term $\big(\sum_{i=1}^{m} u_iB_i\big)x = \big(\sum_{j=1}^{n} x_jN_j\big)u$ with x_j being the jth element of x and $N_j \in \mathbb{R}^{n\times m}$ for $j = i, \ldots, n$.

We now solve the optimal control problem (P1) by Pontryagin's maximum principle. The Hamiltonian of this problem is

$$H(x,u,p) = \frac{1}{2}u^TRu + p^T\Big\{Ax + \Big[B + \Big(\sum_{j=1}^{n} x_jN_j\Big)\Big]u + g\Big\},$$

where $p(t) \in \mathbb{R}^n$ is the co-state vector. The optimal control is then obtained by the necessary condition, $\frac{\partial H}{\partial u} = 0$ (since the control u is unconstrained), given by

$$u^* = -R^{-1}\Lambda^T p, \tag{2}$$

where $\Lambda = B + \sum_{j=1}^{n} x_jN_j$, and the optimal trajectories of the state x and the co-state p satisfy, for $t \in [0, t_f]$,

$$\dot{x}_i = \big[Ax\big]_i - \Big[\Lambda R^{-1}\Lambda^T p\Big]_i + g_i, \tag{3}$$

$$\dot{p}_i = -\big[A^Tp\big]_i + p^T\Big[N_iR^{-1}\Lambda^T + \Lambda R^{-1}N_i^T\Big]p, \tag{4}$$

with the boundary conditions $x(0) = x_0$ and $p(t_f) = 2(x(t_f) - x_d)$ from the transversality condition, where x_i, p_i and $[\,\cdot\,]_i$, $i = 1, \ldots, n$, are the ith component of the respective vectors. By the following change of variables,

$$\tilde{A}_{ij} = A_{ij} - \Big[\Big(N_jR^{-1}\Lambda^T + \Lambda R^{-1}N_j^T\Big)p\Big]_i, \tag{5}$$

$$\tilde{O} = BR^{-1}B^T - \Big(\sum_{j=1}^{n} x_jN_j\Big)R^{-1}\Big(\sum_{j=1}^{n} x_jN_j\Big)^T, \tag{6}$$

we can rewrite (3) and (4) into the form

$$\dot{x} = \tilde{A}x - \tilde{O}p + g, \qquad x(0) = x_0, \tag{7}$$

$$\dot{p} = -\tilde{A}^Tp, \qquad p(t_f) = 2(x(t_f) - x_d), \tag{8}$$

which are in the similar form, with an additional inhomogeneous term g, of the canonical equations that characterize the optimal trajectories of the LQR problem (Anderson & Moore, 1990).

2.1. Iteration procedures

If the matrices $\tilde{A}$ and $\tilde{O}$ in (5) and (6), respectively, were known, then the two-point boundary value problem (TPBVP) described in (7) and (8) can be solved numerically, e.g., by shooting methods (von Stryk & Bulirsch, 1992). However, $\tilde{A}(x,p)$ and $\tilde{O}(x)$ are state dependent, so that this TPBVP is not straightforward to solve. To overcome this, we propose to solve it in an iterative manner by considering the iteration equations

$$\dot{x}^{(k)} = \tilde{A}^{(k-1)}x^{(k)} - \tilde{O}^{(k-1)}p^{(k)} + g, \tag{9}$$

$$\dot{p}^{(k)} = -(\tilde{A}^{(k-1)})^Tp^{(k)}, \tag{10}$$

with the boundary conditions $x^{(k)}(0) = x_0$ and $p^{(k)}(t_f) = 2(x^{(k)}(t_f) - x_d)$ for all iterations $k = 0, 1, 2, \ldots$, where the matrices $\tilde{A}^{(k-1)}(x^{(k-1)}, p^{(k-1)})$ and $\tilde{O}^{(k-1)}(x^{(k-1)})$ are time-varying and defined according to (5) and (6), given by

$$\tilde{A}_{ij}^{(k)} = A_{ij} - \Big[(N_jR^{-1}(\Lambda^{(k)})^T + \Lambda^{(k)}R^{-1}N_j)p^{(k)}\Big]_i, \tag{11}$$

$$\tilde{O}^{(k)} = BR^{-1}B^T - \Big(\sum_{j=1}^{n} x_j^{(k)}N_j\Big)R^{-1}\Big(\sum_{j=1}^{n} x_j^{(k)}N_j\Big)^T, \tag{12}$$

with $\Lambda^{(k)} = B + \sum_{j=1}^{n} x_j^{(k)}N_j$. In order to solve for (9) and (10), we let

$$p^{(k)}(t) = K^{(k)}(t)x^{(k)}(t) + s^{(k)}(t), \tag{13}$$