Constrained Bilinear Systems

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Abstract

In this paper, we study some model control problems which arise in connection with optimal manipulation of dissipative quantum dynamics. It is shown that the problem of optimal control of quantum mechanical phenomenon in presence of dissipation can be reduced to the study of optimization problems associated with a class of constrained Bilinear control systems. These Bilinear systems $\dot{x} = (A + \sum_i^n u_i B_i)x$ are characterized by the fact that the controls can be expressed as polynomial functions of fewer parameters, i.e. $u_i = g_i(v_1, v_2, \ldots, v_k)$ where g_i are polynomials and $k < n$. A general study of these systems is expected to find immediate applications in coherent control of quantum mechanical phenomenon.

1 Introduction

Consider the dynamical system

$$\frac{d}{dt}\begin{bmatrix} r_1 \\ r_2 \end{bmatrix} = \begin{bmatrix} -\alpha u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\alpha u_2^2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix};$$

Given $(r_1(0), r_2(0)) = (1, 0)$, find the optimal control $0 \leq u_1(t), u_2(t) \leq 1$, such that at the terminal time T, $r_2(T)$ is maximized. Problems of this nature arise naturally in the optimal control of quantum mechanical phenomenon in presence of dissipation. These systems are linear in the state and controls can be expressed as polynomial functions of fewer parameters. In this paper we study some optimal control problems related to these systems.

According to the postulates of quantum mechanics, the evolution of the state of a closed quantum system is unitary and is governed by Schrödinger equation. This evolution can be controlled by systematically changing the Hamiltonian of the system. The control of quantum systems has important applications in physics and chemistry. In particular, the ability to steer the state of a quantum system (or of an ensemble of quantum systems) from a given initial state to a desired target state forms the basis of spectroscopic techniques such as nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectroscopy and in the field of laser coherent control and quantum computing. However, in all applications involving control and manipulation of quantum mechanical phenomenon, the system of interest is open, i.e. interacts with its environment (also termed lattice). This undesirable interaction with an external heat bath destroys phase correlations in the quantum system and relaxes the system to its equilibrium state. Manipulating quantum mechanical phenomenon in a manner that minimizes decoherence effects, is a practical problem, in the whole field of coherent spectroscopy and coherent control of quantum mechanical phenomenon.

In this paper, we study some model control problems which arise in connection with optimal manipulation of dissipative spin dynamics in NMR spectroscopy. In the field of NMR spectroscopy, sequences of radio-frequency (RF) pulses with well defined frequencies, amplitudes, phases, and durations are used to manipulate ensembles of spin systems. Applications range from NMR spectroscopy of biological macro molecules to the experimental implementation of quantum-computing algorithms. From a control perspective, the goal in these applications is to steer the state of the spin system using the free-evolution Hamiltonian of the spin system (representing internal system dynamics) and using RF pulse sequences as control variables. Pulse-sequences should be designed to minimize the effects of relaxation or decoherence that are always present in practice. High relaxation or dissipation rates is a major bottleneck in NMR spectroscopy of large proteins. Therefore, developing methods for optimal control of quantum mechanical systems, which minimize dissipation effects is expected to have immediate impact on the field of coherent control of quantum mechanical systems.

The paper is organized as follows. In the following section we recapitulate the basics of quantum mechanics and dissipation in open quantum mechanical systems. In section 3, we look at the model problem of optimal control of coupled two spin system in presence of decoherence. We develop the main ideas presented in this paper through this example.

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2 Control of Dissipative Quantum Dynamics

The state of a closed quantum system, represented by a vector $|\psi\rangle$, evolves unitarily, according to Schrödinger equation

$$\frac{d|\psi(t)\rangle}{dt} = -iH(t)|\psi(t)\rangle, \qquad (1)$$

where $H(t)$ is the Hamiltonian of the system. In this paper, we will only be concerned with finite-dimensional quantum systems. We can split the Hamiltonian as $H = H_d + \sum_{j=1}^{m} u_j(t)H_j$, where H_d is the part of Hamiltonian that is internal to the system and we call it the drift or free evolution Hamiltonian and $\sum_{j=1}^{m} u_j(t)H_j$, is the part of the Hamiltonian that can be externally changed. It is called the control or RF Hamiltonian. In this paper, we will focus on optimal control of ensembles of nuclear spins in NMR spectroscopy. The state of an ensemble of quantum mechanical systems is represented by its density matrix. Given an ensemble of quantum systems with the state vectors given by $|\psi_k\rangle$, $k = 1, \ldots, N$, respectively, the density matrix ρ is defined as

$$\rho = \frac{1}{N}\sum_{k=1}^{N} |\psi_k\rangle\langle\psi_k|,$$

where $\langle\psi_k|$ is the conjugate transpose of the vector $|\psi_k\rangle$. The density matrix of a closed quantum system then evolves as

$$\dot{\rho} = -i[H(t), \rho],$$

where $[,]$ is the matrix commutator. We will refer to the eigenvectors of H_d as the energy eigenstates.

For open quantum systems, the evolution of the system is no longer unitary. The density matrix of the system at any time t is related to the initial state $\rho(0)$ by a trace preserving map [1]

$$\rho(t) = \sum_k E_k(t)\rho(0)E_k^{\dagger}(t), \qquad (2)$$

such that $\sum_k E_k(t)^{\dagger}E_k = I$ (The operators E_k are termed as Kraus operators). In general, it is not possible to write an evolution equation in time for the Kraus operators and hence the density matrix. However, in many practical applications of interest, the lattice can be approximated as an infinite thermostat, whose own state never changes. This assumption is also called Markovian approximation and under these assumptions, it is possible to write the evolution of the density matrix of the system alone in the form (Lindblad Form) [2]

$$\dot{\rho} = [-iH(t), \rho] + L(\rho), \qquad (3)$$

where the term $L(\rho)$ models dissipation or relaxation. The relaxation term $L(\rho)$ is linear in ρ and has the general form

$$L(\rho) = \sum_{\alpha} J_{\alpha}[V_{\alpha}\rho V_{\alpha}^{\dagger} - \frac{1}{2}V_{\alpha}^{\dagger}V_{\alpha}\rho - \frac{1}{2}\rho V_{\alpha}^{\dagger}V_{\alpha}], \qquad (4)$$

where V_{α} are the relaxation super-operators and represent various relaxation mechanisms (Once a basis is chosen, V_{α} are just finite dimensional matrices.)

Relaxation phenomenon is broadly classified into two categories. Adiabatic relaxation (decoherence) and non-adiabatic relaxation(dissipation). Let ρ_D be a density matrix which is diagonal in the energy eigenbasis. All the super-operators V_{β} in equation (4) such that

$$[V_{\beta}\rho_D V_{\beta}^{\dagger} - \frac{1}{2}V_{\beta}^{\dagger}V_{\beta}\rho_D - \frac{1}{2}\rho_D V_{\beta}^{\dagger}V_{\beta}] = 0 \qquad (5)$$

constitutes the adiabatic relaxation or the decoherence terms. This mode of relaxation doesn't effect the population of the energy eigenstates as no energy is exchanged between the environment and the system, but phase correlations between energy eigenstates is destroyed (represented by off diagonal terms in the density matrix when expressed in energy eigenstates). The super-operators V_{β} for which equation (5) is not satisfied, constitute non-adiabatic mode of relaxation in the system and brings the populations to equilibrium, while destroying off diagonal terms in the density matrix. Energy is exchanged between the system and the lattice.

Let us write equation (3) in a more control theoretic notation. We choose energy eigensates as the basis for our Hilbert space. Observe equation (3) is linear in ρ. We expand ρ, as a vector of length n^2 and call it x, with the first n entries of x as the diagonal entries of ρ. Let e_i denote the vector of length n^2 which is one in the i^{th} position and zero everywhere else. In this representation, $e_1, e_2, \ldots,\ e_n$ correspond to density matrices corresponding to energy eigenstates. In this representation we can write the Lindblad equation (3) in the form (Note, the following equation is not the most general form, as we assume that relaxation doesn't couple the diagonal and off diagonal terms of density matrix)

$$\frac{dx}{dt} = (\begin{bmatrix} A & 0 \\ 0 & D \end{bmatrix} + \sum_{i}^{m} u_i \begin{bmatrix} 0 & B_i \\ -B_i^T & C_i \end{bmatrix})x \qquad (6)$$

Where the $n \times n$ matrix A arises due to the spin-lattice relaxation in the system and is responsible for bringing the populations to equilibrium. In general A is a Q matrix for a continuous time markov chain (columns of A sum to zero and all off diagonal elements are non-negative). In systems, where there is no spin-lattice relaxation, the term A is zero. The term D can further be decomposed as $D = D_1 + D_2$. Where $D_1 = D_1^T$ is

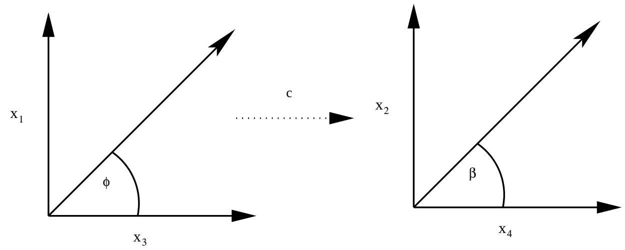

Figure 1:

a negative semi-definite matrix and arises due to decoherence and dissipation. The term $D_2 = -D_2^T$ and arises due to H_d, the drift Hamiltonian of the system. The terms

$$\begin{bmatrix} 0 & B_i \\ -B_i^T & C_i \end{bmatrix},$$

where $C_i = -C_i^T$, correspond to control Hamiltonians. The model problem addressed in the paper is: starting from initial population state $x = e_1$, what is the largest achievable value of $< x, e_k >$ for $k \in 2, \ldots, n$ in both infinite and some prescribed finite time T.

3 Optimal Control of Spin Dynamics in Presence of Decoherence

Our focus, in this paper is on the relaxation phenomenon in the liquid state NMR spectroscopy. The case in which we are interested is well modeled as system consisting of two weakly interacting parts: the spin system consisting of all spin degrees of freedom of the nuclei, and the lattice consisting of all other degrees of freedom of the liquid sample, associated with the molecular rotations and translations. Molecules in solution are constantly being bombarded with solvent molecules and undergo random "Brownian" motion as a result. This stochastic Brownian motion is the principle mechanism of relaxation in NMR spectroscopy. This small inter-collision time of the order of $10^{-14} - 10^{-12}$ seconds, ensures that the correlations between the spin system and the bath decay much faster than the evolution of the spin system and a Markovian approximation is a valid assumption.

We analyze an optimization problem related to optimal control of two coupled spins under relaxation [3]. The control theoretic issues are captured by the following problem. Consider the control system

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 & u & 0 \\ 0 & 0 & 0 & v \\ -u & 0 & -d & -c \\ 0 & -v & c & -d \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \quad (7)$$

The objective is to find out that starting with the state $e_1^T = (1, 0, 0, 0)$, what is the maximum achievable value of x_2 and what are the optimal controls u and v that achieve this value. Observe if u and v are set to 0 then the initial state e_1 doesn't evolve at all and there is no build up of x_2. However by switching on u it is possible to rotate x_1 to x_3 which evolves to x_4 under the skew symmetric matrix $\begin{bmatrix} 0 & -c \\ c & 0 \end{bmatrix}$ and dissipates under the term $\begin{bmatrix} -d & 0 \\ 0 & -d \end{bmatrix}$. The state x_4 can then be rotated to x_2 by switching the controls v. The goal is to find the optimal u and v as a function of time which produce the maximum value of x_2.

By switching on the control u, the initial state e_1 can be transformed to any state of the form $e_1 \sin\phi + e_3 \cos\phi$ in almost no time. Let $r_1^2(t) = x_1^2(t) + x_3^2(t)$ and $r_2^2(t) = x_2^2(t) + x_4^2(t)$. Using the control u, we can exactly control the angle ϕ in the term $r_1(t)\cos\phi\, e_3 + r_1(t)\sin\phi\, e_1$. Now observe the vector e_1 doesn't evolve but the vector e_3 evolves to e_4 under the coupling c and also dissipates. As the vector e_4 is produced, its magnitude begins to decay too. By use of control v we can rotate e_4 to e_2 and exactly control the angle β in the term $r_2(t)\sin\beta\, e_2 + r_2(t)\cos\beta\, e_4$ (See Fig. 1). We can now write an equation for $r_1(t)$ and $r_2(t)$ and it takes the form

$$\frac{d}{dt}\begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} = \begin{bmatrix} -d\cos^2\phi & -c\cos\phi\cos\beta \\ c\cos\phi\cos\beta & -d\cos^2\beta \end{bmatrix}\begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} \quad (8)$$

where ϕ and β can be explicitly controlled using controls u and v. Denoting $u_1 = \cos\phi$ and $u_2 = \cos\beta$, and dilating time by a factor of c, we can rewrite the above equations as

$$\frac{d}{dt}\begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} = \begin{bmatrix} -\alpha u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\alpha u_2^2 \end{bmatrix}\begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix}. \quad (9)$$

Here u_1 and u_2 are control parameters, which take there values between -1 and 1 and $\alpha = d/c$. For the dynamical system in equation (9), how should $u_1(t)$ and $u_2(t)$ be chosen so that starting from $r_1(0) = 1$ we achieve the largest value for r_2. To understand qualitativly the optimization problem here, observe if $\alpha = 0$ (no decoherence), then by putting $u_1(t) = u_2(t) = 1$, we get $r_2(\frac{1}{2}) = 1$, and we get the full transfer. However if $\alpha \neq 0$, then it is not the best strategy to keep $u_1(t)$ and $u_2(t)$ both 1, because although this rotates the vector (r_1, r_2) from $(1, 0)$ to $(0, 1)$ rapidly, it increases dissipation in the system. This is depicted in trajectory a in the figure 2. Using maximum principle, we will obtain analytical expression for the largest achievable value of r_2 and the optimal values of $u_1(t)$ and $u_2(t)$. Curve b in figure 2 shows the optimal trajectory if $u_1(t)$ and $u_2(t)$ are chosen optimally. This leads to higher transfer efficiency from r_1 to r_2.

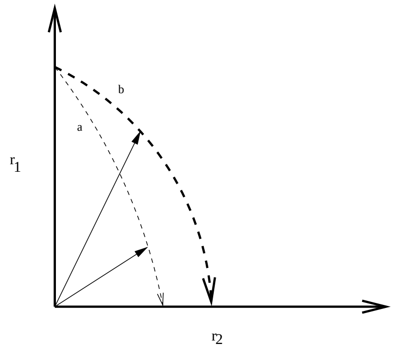

Figure 2: The curve a shows the trajectory of dynamical system 9 when $u_1 = u_2 = 1$ and $\alpha = 1$. Curve b showns the trajectory of dynamical system 9 for optimal choice of u_1 and u_2 and $\alpha = 1$. The optimal trajectory approaches the r_2 axis at the point $(r_1, r_2) = (0, \sqrt{2} - 1)$.

Problem 1 Consider the dynamical system

$$\frac{d}{dt}\begin{bmatrix} r_1 \\ r_2 \end{bmatrix} = \begin{bmatrix} -\alpha u_1^2 & -u_1 u_2 \\ u_1 u_2 & -\alpha u_2^2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}; \qquad (10)$$

Given $(r_1(0), r_2(0)) = (1, 0)$, find the optimal control $(u_1^*(t), u_2^*(t))$, $0 \leq u_1, u_2 \leq 1$, $t \in [0, \infty)$, such that r_2 is maximized.

Theorem 1 For the control system described in problem 1, let

$$\eta = \sqrt{\alpha^2 + 1} - \alpha.$$

Then the optimal feedback control $(u_1^*(r_1, r_2), u_2^*(r_1, r_2))$ satisfy

$$\frac{u_1^*(r_1, r_2)}{u_2^*(r_1, r_2)} = \frac{r_2}{\eta r_1} \qquad (11)$$

and the optimal return function $V(r_1, r_2)$ is

$$V(r_1, r_2) = \sqrt{r_2^2 + r_1^2 \eta^2}. \qquad (12)$$

Proof: We use maximum principle of pontryagin. The Hamiltonian of the system takes the form

$$\mathbb{H} = \lambda_1(-\alpha u_1^2 r_1 - u_1 u_2 r_2) + \lambda_2(u_1 u_2 r_2 - \alpha u_2^2 r_2),$$

where $\lambda_1 = \frac{\partial V}{\partial r_1}$ and $\lambda_2 = \frac{\partial V}{\partial r_2}$ are the costate variables. We introduce the following notation. Let

$$a = \frac{\lambda_2}{\lambda_1}; \quad b = \frac{r_2}{r_1}.$$

The Hamiltonian can then be written as

$$\mathbb{H} = -\lambda_1 r_1[\alpha\ ab\ u_2^2 + (b - a)u_1 u_2 + \alpha u_1^2],$$

The pontryagin's maximum principle states that if u_1^*, u_2^* are optimal control laws then

$$(u_1^*, u_2^*) = \arg\max_{(u_1, u_2)} \mathbb{H}(u_1, u_2) \qquad (13)$$

$$\mathbb{H}(u_1^*, u_2^*) = 0 \qquad (14)$$

Since $a, b > 0$, if $(a - b) \leq 0$, then the only solution to equations (13, 14) is the trivial solution $u_1^* = u_2^* = 0$. Therefore $(a - b) > 0$. Also note, when $(a - b)^2 < 4\alpha^2 ab$, the only solution to equations (13, 14) is again the trivial solution. Suppose $(a - b)^2 > 4\alpha^2 ab$, i.e. $\frac{(a-b)^2}{4\alpha^2} = ab + \kappa$ for $\kappa > 0$. Then

$$\mathbb{H} = -\lambda_1 r_1[\frac{(a - b)}{2\sqrt{\alpha}}\ u_2 - \sqrt{\alpha} u_1]^2 + \kappa \lambda_1 r_1 u_1^2,$$

and hence $\max \mathbb{H} > 0$. Therefore the only case for which (13, 14) can be satisfied is

$$(b - a)^2 = 4ab\alpha^2, \qquad (15)$$

implying

$$\sqrt{\frac{b}{a}} = \sqrt{1 + \alpha^2} - \alpha. \qquad (16)$$

In this regime, maximizing $\mathbb{H}$, we get

$$\frac{u_1^*}{u_2^*} = \frac{a - b}{2\alpha}, \qquad (17)$$

and from (15,16) that

$$\frac{u_1^*}{u_2^*} = \frac{b}{\sqrt{1 + \alpha^2} - \alpha}.$$

Integrating using the optimal control law, we get the optimal return function $V(r_1, r_2) = \sqrt{r_2^2 + r_1^2 \eta^2}$.

Remark 1 It is important to note that the point $(r_1, r_2) = (0, \eta)$, is only reached in the limit of infinite time. Let $\overline{\mathbf{R}((1,0))}$, denote the closure of the reachable set of the point $(1, 0)$. Then $(0, \eta) \in \overline{\mathbf{R}((1, 0))}$. The optimal control policy can be realized as

$$u_2^* = 1 \quad ; \quad u_1^* = \frac{r_2}{\eta r_1}; \quad 0 \leq \frac{r_2}{r_1} \leq \eta;$$

$$u_1^* = 1 \quad ; \quad u_2^* = \frac{\eta r_1}{r_2}; \quad \frac{r_2}{r_1} \geq \eta.$$

Remark 2 Observe that the initial point $(1, 0)$ is a stationary point of the optimal control policy. This optimal policy in the infinite case should then be interpreted as the limit of optimal control policy for the finite time problems as the terminal time T approaches infinity. In theorem 3 we explicitly compute the optimal policy for finite terminal time.

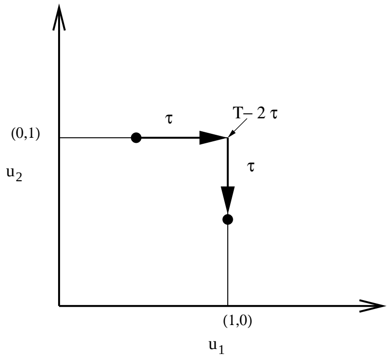

Figure 3:

Remark 3 It is now possible to explicitly characterize the set, $\overline{\mathbf{R}((1,0))}$. In the first quadrant, the closure of the reachable set has the form

$$\overline{\mathbf{R}((1,0))} = \{r_1 \geq 0, r_2 \geq 0 | \sqrt{r_2^2 + r_1^2\eta^2} \leq \eta\}.$$

This is depicted in figure 2. This in turn explicitly characterizes the closure of the reachable set for the control system, described by equation (7) as described in the following theorem.

Theorem 2 For the control system

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 & u & 0 \\ 0 & 0 & 0 & v \\ -u & 0 & -d & -c \\ 0 & -v & c & -d \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix},$$

let $\alpha = d/c$ and $\eta = \sqrt{1+\alpha^2} - \alpha$. Then the closure of the reachable set $\overline{\mathbf{R}((1,0,0,0))}$ is given by

$$\{(x_1, x_2, x_3, x_4) | \sqrt{(x_2^2 + x_4^2) + \eta^2(x_1^2 + x_3^2)} \leq \eta\}.$$

We now consider a finite time version of problem 1.

Problem 2 We now consider a finite time version to the problem 1. For the control system in problem 1, given $(r_1(0), r_2(0)) = (1, 0)$, find the optimal control $(u_1^*(t), u_2^*(t))$, $t \in [0, T]$, such that $r_2(T)$ is maximized.

Remark 4 We first describe qualitatively the nature of optimal trajectoy and optimal control. For given T there is a τ (function of T), such that for $0 \leq t \leq \tau$, $u_2(t) = 1$ while $u_1(t)$ is increased gradually from a value $u_1(0) < 1$ to $u(\tau) = 1$ as described in following

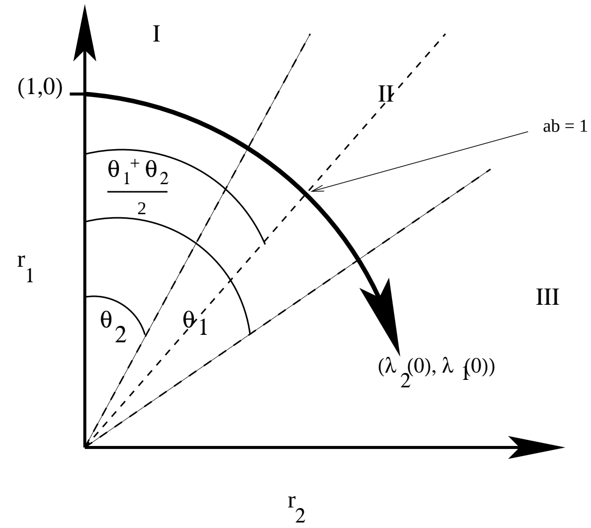

Figure 4:

theorem. Then for time $\tau \leq t \leq T - \tau$, the optimal control $u_1(t) = 1$ and $u_2(t) = 1$. Finally for $t \geq T - \tau$, we have $u_1(t) = 1$ and $u_2(t)$ is decreased from 1 to $u_2(T) = u_1(0)$. The optimal control always satisfies $u_1(t) = u_2(T - t)$. This is depicted in Figure 3. If $\tan T \leq \frac{1}{2\alpha}$, then $\tau = 0$. Figure 4, depicts the optimal trajectory. At time τ, the optimal trajectory makes an angle θ_2 with the r_1 axis and at time $T - \tau$ the optimal trajectory makes an angle θ_1 with the r_1 axis, where θ_1 and θ_2 depend only on T.

Definition 1 For the control system in problem 2, we define $\eta(t) = 1 + 2\alpha^2 - 2\alpha\sqrt{1+\alpha^2}\coth(\sqrt{1+\alpha^2}t + 2\beta)$, where $\sinh(\beta) = \alpha$. Further define $\theta_1(t) = \tan^{-1}\frac{1-\eta(t)}{2\alpha}$ and $\theta_2(t) = \tan^{-1}\frac{2\alpha\eta(t)}{1-\eta(t)}$.

Theorem 3 For the control system in problem 2, the optimal control $u_1^*(t) = u_2^*(T-t)$. If $\tan T \leq \frac{1}{2\alpha}$, then $u_1^*(t) = u_2^*(t) = 1$ and $r_2(T) = \exp(-\alpha T)\sin(T)$. For $\tan T > \frac{1}{2\alpha}$, there exists $\tau \leq \frac{T}{2}$, satisfying

$$T = 2\tau + \theta_1(\tau) - \theta_2(\tau). \qquad (18)$$

The optimal control then satisfies

$$u_2^*(t) = 1\,; \quad t \leq T - \tau \qquad (19)$$

$$u_2^*(t) = \frac{(1 - \eta(T-t))r_1(t)}{2\alpha r_2(t)}; \quad t > T - \tau \qquad (20)$$

The optimal cost

$$r_2(T) = \frac{\exp(-\alpha(T - 2\tau))(1 - \alpha\sin 2\theta_1(\tau))}{\sin(\theta_1(\tau) + \theta_2(\tau))} \qquad (21)$$

Proof: As in theorem 1, the Hamiltonian is expressed as

$$\mathbb{H} = -\lambda_1 r_1[\alpha u_1^2 - (a-b)u_1u_2 + \alpha ab u_2^2].$$

For the finite horizon problem $\max_{u_1,u_2} \mathbb{H} > 0$. This implies $(a-b)^2 > 4\alpha^2 ab$. We consider three separate cases for the problem

1. **Case I:** If $(a-b) < 2\alpha$, then the maximum of $\mathbb{H}$ is obtained for $u_2 = 1$ and $u_1 = \frac{a-b}{2\alpha}$.
2. **Case II:** If $(a-b) \geq 2\alpha$ and $\frac{a-b}{ab} \geq 2\alpha$, then the maximum of $\mathbb{H}$ is obtained for $u_1 = 1$ and $u_2 = 1$.
3. **Case III:** If $\frac{a-b}{ab} < 2\alpha$, then the maximum of $\mathbb{H}$ is obtained for $u_1 = 1$ and $u_2 = \frac{a-b}{2\alpha ab}$.

The adjoint variables (λ_1, λ_2) satisfy the equations,

$$\frac{d}{dt}\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} \alpha u_1^2 & -u_1 u_2 \\ u_1 u_2 & \alpha u_2^2 \end{bmatrix}\begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}, \qquad (22)$$

where $(\lambda_1(T), \lambda_2(T)) = (0, 1)$. Observe $V = \lambda_1 r_1 + \lambda_2 r_2$ is a constant for optimal trajectory and equals the optimal cost $r_2(T) = \lambda_1(0)$. Writing the equation for adjoint variables backward in time, let $\sigma = T - t$ then

$$\frac{d}{d\sigma}\begin{bmatrix} \lambda_2 \\ \lambda_1 \end{bmatrix} = \begin{bmatrix} -\alpha u_2^2 & -u_1 u_2 \\ u_1 u_2 & -\alpha u_1^2 \end{bmatrix}\begin{bmatrix} \lambda_2 \\ \lambda_1 \end{bmatrix},$$

where $(\lambda_2(\sigma), \lambda_1(\sigma))_{\sigma=0} = (1, 0)$. This is exactly the same optimization problem as in equation (10), where λ_1 takes the role of r_2 and λ_2 replaces r_1 and the roles of u_1 and u_2 have been switched. Again u_1 and u_2 should be chosen to maximize $\lambda_1(\sigma)|_{\sigma=T}$. From symmetry, we then have

$$\begin{aligned} u_1^*(t) &= u_2^*(T-t) \\ r_1(t) = \lambda_2(T-t) \quad &; \quad r_2(t) = \lambda_1(T-t) \\ a.b(\frac{T}{2}) = 1 \quad &; \quad V = 2r_1(\frac{T}{2})r_2(\frac{T}{2}) \end{aligned}$$

Observe from (10,22), $ab(t)$ is monotonicaly increasing and since $ab(0) = 0$ and $ab(\frac{T}{2}) = 1$, we have $ab(t) < 1$ for $t < \frac{T}{2}$. Therefore $u_2^*(t) = 1$ for $t < \frac{T}{2}$. Since $b(0) = 0$, depending on $a(0)$ we have two cases.

Case A In this case $\frac{a(0)}{2\alpha} \geq 1$. Then we start in the case II discussed above and verify that in this case $a-b$ is increasing for $ab < 1$. Therefore we stay in this case for all $t \in [0, \frac{T}{2}]$ and therefore $u_1^* = u_2^*(t) = 1$ for all t. Since $b(0) = 0$, we have $b(\frac{T}{2}) = \tan T$. Similarly,

$$a(\frac{T}{2}) = \frac{a(0) + \tan(\frac{T}{2})}{1 - a(0)\tan(\frac{T}{2})}.$$

If $ab(\frac{T}{2}) = 1$ then it implies that $\tan(T) \leq \frac{1}{2\alpha}$.

Case B If $\frac{a(0)}{2\alpha} < 1$, then $u_1^*(0) = \frac{a(0)}{2\alpha}$ and the system begins in case I. Let $\eta(t)$ satisfy

$$\frac{d\eta}{dt} = -\frac{\eta^2 - 2\eta + 1}{2\alpha} + 2\alpha\eta, \quad \eta(0) = 0.$$

The solution to this equation is given by $\eta(t) = 1 + 2\alpha^2 - 2\alpha\sqrt{1+\alpha^2}\coth(\sqrt{1+\alpha^2}t + 2\beta)$, where $\sinh(\beta) = \alpha$. In this case, the optimal trajectory satisfies $\frac{b}{a} = \eta(t)$. After time τ, $\frac{a-b}{2\alpha}$ becomes equal to 1 and the system switches to case II. Putting $\frac{a-b}{2\alpha} = 1$ and $\frac{b}{a} = \eta(t)$, we get

$$\frac{r_2(\tau)}{r_1(\tau)} = \frac{2\alpha\eta(\tau)}{1 - \eta(\tau)}.$$

Then again by symmetry at time $T-\tau$ we have $\frac{1}{2\alpha}(\frac{1}{b} - \frac{1}{a}) = 1$ and the system switches from case II to case III. In case III, verify $b = a\eta(T-t)$ and the switching to this case occurs at $\frac{r_2}{r_1} = \frac{1-\eta(\tau)}{2\alpha}$. Thus the system spends $T - 2\tau$ in region II. Then we have

$$T - 2\tau = \tan^{-1}\frac{1-\eta(\tau)}{2\alpha} - \tan^{-1}\frac{2\alpha\eta(\tau)}{1-\eta(\tau)}.$$

Thus providing result (18). The optimal control $u_2^*(t)$ then satisfies (19) and (20).

We now derive an explicit expression for $r_2(T)$. For $t \geq T - \tau$,

$$V(t) = \sqrt{r_1^2(t) + \eta(T-t)r_2^2(t)},$$

is constant along the system trajectories and equals the optimal return function $r_2(T)$. At $t = T - \tau$, we have $\frac{r_2(T-\tau)}{r_1(T-\tau)} = \tan\theta_1 = \frac{1-\eta(\tau)}{2\alpha}$ and therefore

$$V(t) = R_1\sqrt{\sin^2\theta_1 + \cos^2\theta_1 - 2\alpha\sin\theta_1\cos\theta_1}, \quad (23)$$

where $R_1 = \sqrt{r_1^2(T-\tau) + r_2^2(T-\tau)}$. Also note $V(\frac{T}{2}) = 2r_1(\frac{T}{2})r_2(\frac{T}{2})$. At time $t = \frac{T}{2}$, we then have $\frac{r_2}{r_1} = \tan(\frac{\theta_1+\theta_2}{2})$ (see Fig 4) and therefore

$$V(\frac{T}{2}) = R_2^2\sin(\theta_1 + \theta_2) \qquad (24)$$

where $R_2 = \sqrt{r_1^2(\frac{T}{2}) + r_2^2(\frac{T}{2})}$. Note between $\frac{T}{2}$ and $T-\tau$, the system evolves under $u_1 = u_2 = 1$. Therefore $R_1 = R_2\exp(-(\frac{T}{2} - \tau))$. Equating (23) and (24), we get equation (21).

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