Semidefinite Programming and Reachable Sets of Dissipative Bilinear Control Systems

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Abstract

In this manuscript, we investigate optimal control problems which arise in connection with manipulation of dissipative quantum dynamics. These problems motivate the study of a class of dissipative bilinear control systems. For these systems it is shown that the optimal solution and the reachable set can be found by solving a semidefinite program. In practice, solutions to these problems generate optimal methods for control of quantum mechanical phenomena in presence of dissipation. In the area of coherent spectroscopy, this translates into the maximum signal to noise ratio that can be obtained in a spectroscopy experiment.

1 Introduction-Statement of the Problem

Consider the following optimal control problem. Given the dynamical system below

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{y}_1 \\ \dot{y}_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -v_1 & 0 \\ 0 & 0 & 0 & -v_2 \\ v_1 & 0 & -k & -J \\ 0 & v_2 & J & -k \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ y_1 \\ y_2 \end{bmatrix}$$
(1)

and starting from the initial state $e_1 = (1, 0, 0, 0)^T$, what is the maximum achievable value of x_2 and what are the optimal controls $v_1(t) \in \Re$ and $v_2(t) \in \Re$ that achieve this value? Problems like this are associated with optimal manipulation of quantum mechanical phenomena under dissipation.

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Specifically, the optimization problem stated above comes from Nuclear Magnetic Resonance (NMR) spectroscopy and is related to optimal control of two coupled spins in presence of transverse relaxation [1]. The state variables x_i, y_i represent averages of various quantum mechanical spin operators. The available controls $v_1(t)$ and $v_2(t)$ correspond to the components of the magnetic field in the NMR experimental setup. Parameter k > 0 expresses the transverse relaxation rate while J is the coupling constant between the spins.

Observe that if v_1 and v_2 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 turning on v_1 , it is possible to rotate x_1 to y_1 , see Fig. 1. This evolves to y_2 under the skew symmetric matrix

$$\left[\begin{array}{cc} 0 & -J \\ J & 0 \end{array}\right] ,$$

while both y_1 and y_2 dissipate under the term

$$\left[\begin{array}{cc} -k & 0\\ 0 & -k \end{array}\right]$$

The state y_2 can then be rotated to x_2 by switching on the control v_2 . We want to find the optimal v_1 and v_2 that maximize the value of x_2 . It is intuitively clear that no matter how large we make $v_1(t), v_2(t)$, the transfer $x_1 \to x_2$ cannot be done without any loss, since the intermediate transfer $y_1 \to y_2$ is entirely due to internal dynamics over which there is no control, thus there is an unavoidable dissipation because of k > 0.

Define

$$r_i = \sqrt{x_i^2 + y_i^2} \ . \tag{2}$$

Using (1), evolution equations for r_1, r_2 can be found. We get the system

$$\begin{bmatrix} \dot{r}_1 \\ \dot{r}_2 \end{bmatrix} = \begin{bmatrix} -k\cos^2\phi_1 & -J\cos\phi_1\cos\phi_2 \\ J\cos\phi_1\cos\phi_2 & -k\cos^2\phi_2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix},$$

where $\cos \phi_1 = y_1/r_1$, $\cos \phi_2 = y_2/r_2$, see Fig. 1. Using the control v_1 which rotates x_1 to y_1 , we can control the angle ϕ_1 . Analogously, using v_2 which rotates y_2 to x_2 , we can control the angle ϕ_2 . Denoting $u_1 = \cos \phi_1$, $u_2 = \cos \phi_2$ and dilating time by a factor of J, the above system can be rewritten as

$$\begin{bmatrix} \dot{r}_1 \\ \dot{r}_2 \end{bmatrix} = \begin{bmatrix} -\xi u_1^2 & -u_1 u_2 \\ u_2 u_1 & -\xi u_2^2 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} .$$
(3)

Here u_1 and u_2 are control parameters which take their values in the interval [-1, 1] and $\xi = k/J$. The initial problem of maximum transfer from x_1 to x_2 has been transformed to the following equivalent question:

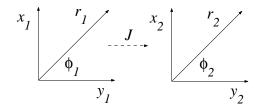


Figure 1: Schematic representation of the evolution of system (1). Control v_1 rotates x_1 to y_1 . Under the *J* coupling y_1 evolves to y_2 , while both dissipate because of the relaxation term *k*. Control v_2 rotates y_2 to x_2 . The new state variables r_1, r_2 , defined by (2), are also shown. The corresponding new control parameters are $u_1 = \cos \phi_1, u_2 = \cos \phi_2$.

Given the dynamical system (3) and the initial state $(r_1(0), r_2(0)) = (1, 0)$, find the optimal control $(u_1(t), u_2(t)), |u_1|, |u_2| \leq 1$, such that r_2 is maximized.

Note that once r_2 is maximized, the control v_2 can be used to transfer it to x_2 with no loss, so the above question is indeed equivalent to the original problem.

Motivated by this example, which originates from a real physical system, let us consider the following n-dimensional generalization of system (1):

$$\begin{bmatrix} \dot{x} \\ \dot{y} \end{bmatrix} = \begin{bmatrix} 0 & -V \\ V & A \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} , \tag{4}$$

where $x = (x_1, x_2, \ldots, x_n)^T$, $y = (y_1, y_2, \ldots, y_n)^T$, $V = \text{diag}(v_1, v_2, \ldots, v_n)$ and $A = \{a_{ij}\}$ is such that its symmetric part $A + A^T$ is negative definite. This condition insures that the norm of the vector (x, y) can only decrease. This models the physics in open quantum systems, where dissipation can only reduce coherence in the system dynamics. Furthermore, A is such that any two states y_i and y_j are coupled by its off-diagonal elements, not necessarily directly (we say A is *irreducible*).

Problem 1 Given the dynamical system (4) and the starting state (x(0), y(0)), find the optimal control $(v_1(t), v_2(t), \ldots, v_n(t))$ which maximizes x_n .

It is shown in the following section that the negative definiteness condition on A is a sufficient condition for the existence of an optimal solution. If we define $r_i = \sqrt{x_i^2 + y_i^2}$ and work as in the 2-dimensional case, we find that r_i satisfies the equation

$$\frac{dr_i}{dt} = \sum_{j=1}^n a_{ij} u_i u_j r_j , \qquad (5)$$

where $u_i = y_i/r_i$. Problem 1 has been transformed to the following.

Problem 2 Given the dynamical system defined by (5) for i = 1, 2, ..., n, with $A = \{a_{ij}\}$ irreducible and such that $A + A^T$ negative definite, and the starting state $(r_1(0), r_2(0), ..., r_n(0))$, with $r_i(0) \ge 0$, find the optimal control $(u_1(t), u_2(t), ..., u_n(t))$, $|u_i| \le 1$, which maximizes r_n , while it preserves $r_i(t) \ge 0$.

Observe that if $T_1 < T_2$, then the maximum achievable value in time T_1 cannot exceed the corresponding value in time T_2 , since by putting $u_i = 0$ the evolution in the interval $(T_1, T_2]$ can be stopped. Therefore, Problem 2 is considered as an *infinite horizon problem*.

Multiplying the i^{th} equation of system (5) with $2r_i$, we get

$$\frac{d}{dt}\left(r_i^2\right) = \sum_{j=1}^n 2a_{ij}u_iu_jr_ir_j \tag{6}$$

and from this

$$\frac{d}{dt}\left(r_i^2\right) = U^2 \sum_{j=1}^n 2a_{ij} \frac{u_i r_i}{U} \frac{u_j r_j}{U} , \qquad (7)$$

where

$$U = \sqrt{\sum_{i=1}^{n} (u_i r_i)^2} .$$
 (8)

By setting

$$p_i = r_i^2, \qquad m_i = \frac{u_i r_i}{U}, \qquad (9)$$

and rescaling time according to $dt' = U^2 dt$, equation (7) becomes

$$\frac{dp_i}{dt'} = \sum_{j=1}^n 2a_{ij}m_i m_j \;. \tag{10}$$

The initial optimal control problem has been transformed to the following one.

Problem 3 Given the dynamical system defined by (10) for i = 1, 2, ..., nand the starting point $p(0) = (p_1(0), p_2(0), ..., p_n(0))^T$, $p_i(0) \ge 0$, find the unit vector $m(t') = (m_1(t'), m_2(t'), ..., m_n(t'))^T$ that maximizes p_n , while it preserves $p_i(t') \ge 0$. Matrix $A = \{a_{ij}\}$ is irreducible and such that $A + A^T$ is negative definite.

Note that, although Problem 2 is an infinite horizon problem, Problem 3 defined above may achieve its maximum for a finite final time T_f . There is no inconsistency here, since the times for the two systems are related through $dt' = U^2 dt$, so $T_f = \int_0^{T_f} dt' = \int_0^\infty U^2 dt$. If $U(t) \to 0$ sufficiently fast as $t \to \infty$, then T_f is finite. As we will see, this is indeed the case.

In the following, we study problems 2 and 3 in detail. Having found an optimal solution for the latter, we can easily find a corresponding optimal control law for the former. The structure of the paper is as follows. In section 2, it is shown that the solution of Problem 3 can be reduced to the solution of a semidefinite program and that the negative definiteness of the symmetric part of A is a sufficient condition for the existence of an optimal solution. It is also shown how the semidefinite programming formalism can be used for calculating reachable sets. In section 3, some useful existent results regarding the rank of matrices that solve our semidefinite program are presented. These results are used in section 4, where some specific examples are examined. The examples include system (3) and another system which again arises from an optimal control problem of spin dynamics in NMR spectroscopy.

2 Reduction to a Semidefinite Program

In the following, the inner product $\langle \cdot, \cdot \rangle$ in the space of symmetric $n \times n$ matrices Sym_n is defined in the usual way as the trace of the matrix product, i.e. $\langle A, B \rangle = \operatorname{tr}(AB)$ for $A, B \in \operatorname{Sym}_n$. Note also that $A \succeq 0$ denotes that matrix $A \in \operatorname{Sym}_n$ is positive semidefinite, $A \prec 0$ that is negative definite etc.

Theorem 1 Let us define matrices $A_i \in Sym_n, i = 1, 2, ..., n$, by the relation

$$A_{i} = \begin{bmatrix} a_{i1} & & & \\ O_{i1} & \vdots & O_{i2} & \\ a_{i(i-1)} & & & \\ a_{i1} & \dots & a_{i(i-1)} & 2a_{ii} & a_{i(i+1)} & \dots & a_{in} \\ & & & a_{i(i+1)} & \\ O_{i3} & \vdots & O_{i4} & \\ & & & a_{in} & \end{bmatrix}$$

where a_{ij} are the elements of matrix A given in Problem 3 and O_{il} , l = 1, 2, 3, 4, are zero matrices with appropriate sizes. The solution of Problem 3 can be reduced to the solution of the following semidefinite program:

Find
$$\mathcal{E} = \max_{M} \langle A_n, M \rangle$$

subject to $\langle A_i, M \rangle = -p_i(0), \quad i = 1, 2, \dots, n-1$
and $M \succeq 0$.

The maximum achievable value of p_n is $p_n(0) + \mathcal{E}$.

Proof: Let T_f be the time when p_n achieves its maximum, i.e. the final time. From equation (10) it is

$$p_i(T_f) = p_i(0) + \sum_{j=1}^n 2a_{ij} \int_0^{T_f} m_i(t')m_j(t')dt' .$$
(11)

Observe that if we define the positive semidefinite matrix M through the relation

$$M = \int_0^{T_f} m(t') m^T(t') dt' , \qquad (12)$$

then (11) becomes

$$p_i(T_f) = p_i(0) + \langle A_i, M \rangle .$$
(13)

One other important observation is that the end point of the optimal trajectory should lie on the line $(0, 0, \ldots, 0, p_n)$ in *p*-space. Suppose that the end point has a component $p_k > 0$ for some $k \neq n$. If p_k is directly coupled to p_n then choose $m = (0, 0, \ldots, 0, m_k, 0, \ldots, 0, m_n)^T$ such that $m_n(a_{nk}m_k + a_{nn}m_n) > 0$ and evolve the system until $p_k = 0$. Thereby we get a greater value of p_n . If p_k is not directly coupled to p_n , we can still transfer from p_k to p_n using intermediate states (because matrix A is irreducible). We conclude that at the final time T_f the end point of the optimal trajectory should lie on the line $(0, 0, \ldots, 0, p_n)$. Thus, we have to maximize $p_n(T_f) = p_n(0) + \langle A_n, M \rangle$ under the conditions $p_i(T_f) = p_i(0) + \langle A_i, M \rangle = 0$, $i = 1, 2, \ldots, n - 1$. Equivalently, we have to solve the following semidefinite program: Find $\mathcal{E} = \max_M \langle A_n, M \rangle$ subject to $\langle A_i, M \rangle = -p_i(0)$ for $i = 1, 2, \ldots, n - 1$ and $M \succeq 0$.

Having found an optimal M, we can always find an appropriate unit vector m(t') such that $M = \int_0^{T_f} m(t')m^T(t')dt'$ and $p_i(t') \ge 0$. Since $M \succeq 0$, it can always be decomposed in the form

$$M = \sum_{k=1}^r \lambda_k \mathbf{m}_k \mathbf{m}_k^T \; ,$$

where λ_k are the positive eigenvalues of M, \mathbf{m}_k are the corresponding (real) normalized eigenvectors and r is the rank of M. Now let N be a positive integer. Rewrite the above relation in the form

$$M = N \sum_{k=1}^{r} \Delta \lambda_k \mathbf{m}_k \mathbf{m}_k^T ,$$

where $\Delta \lambda_k = \lambda_k / N$, and define the times t'_k through

$$t'_0 = 0$$
, $t'_k = \sum_{l=1}^k \Delta \lambda_l$ for $k = 1, 2, \dots, r$.

Let us forget for a moment the restrictions $p_i(t') \ge 0$. If we apply the control

$$m(t') = \mathbf{m}_k$$
 for $t'_{k-1} \le t' < t'_k$, $k = 1, 2, \dots, r$

and repeat for N times, then on the one hand the requirement

$$\int_0^{T_f} m(t')m^T(t')dt' = M$$

is satisfied and on the other hand the trajectory in *p*-space approximates the line joining the initial point $I(p_1(0), p_2(0), \ldots, p_n(0))$ to the final point $F(0, 0, \ldots, p_n(T_f))$, see Fig 2(a). If N is large enough then the trajectory actually follows this line, see Fig. 2(b), thus the restrictions $p_i(t') \ge 0$ are satisfied. Note that $T_f = \sum_{k=1}^r \lambda_k = \operatorname{tr}(M)$ is finite, if $\operatorname{tr}(M) < +\infty$. In the special case where r = 1, it is $M = \lambda \mathbf{mm}^T$ and thus $m(t') = \mathbf{m}$ for $t' \in [0, T_f], T_f = \lambda$.

The conclusion is that we just need to solve the semidefinite program defined above. The maximum achievable value of p_n is $p_n(T_f) = p_n(0) + \mathcal{E}$.

We show next how this control law can be applied to system (5) in Problem 2. For $0 \le t' \le t'_1$, $m(t') = \mathbf{m}_1 = \text{constant}$. Since, additionally, \mathbf{m}_1 is a unit vector, we can assume without loss of generality that its first component $m_1 \ne 0$. Consider the ratios

$$\frac{u_i r_i}{u_1 r_1} = \frac{m_i(t')}{m_1(t')} = s_i , \quad i = 1, 2, \dots, n.$$

For $0 \le t' \le t'_1$, s_i are constant. Define

$$\mathcal{M} = \max_{i} \left(\left| \frac{s_i r_1}{r_i} \right| \right), \quad i = 1, 2, \dots, n.$$

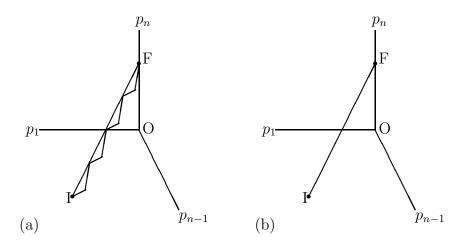


Figure 2: (a) Trajectory in *p*-space following the control law presented in the text, for r = 2 and N = 4. It approximates the straight line from the initial point *I* to the final point *F*. Note that the restrictions $p_i(t') \ge 0$ may not be satisfied when *N* is small (b) For large *N* the trajectory coincides with the line *IF*, so the restrictions $p_i(t') \ge 0$ are satisfied.

The optimal policy can be realized as

$$u_1 = \frac{1}{\mathcal{M}}$$

and

$$u_i = \frac{s_i r_1}{r_i} u_1 \; ,$$

where i = 2, 3, ..., n. With the above choice we insure that $|u_i| \leq 1$. Using this feedback law we can evolve system (5) in time t and calculate the function $U(t) = \sum_{i=1}^{n} (u_i r_i)^2$. Then, we can find $t' = \int_0^t U^2 dt$. When $t' = t'_1$, we switch to $m(t') = \mathbf{m}_2$ and repeat the above procedure. If the rank of M is r = 1then the ratios s_i keep the same value for all times. Note that the maximum achievable value of r_n is

$$r_n(\infty) = \sqrt{p_n(T_f)} = \sqrt{p_n(0) + \mathcal{E}} = \sqrt{r_n^2(0) + \mathcal{E}} .$$
(14)

In the above discussion we implicitly assumed that an optimal solution exists, and we used for \mathcal{E} the characterization "maximum" instead of the more formal "supremum". We show below that the negative definiteness of $A + A^T$ is a sufficient condition for the existence of an optimal solution. The following lemma is used.

Lemma 1 If $B \succ 0$ and $M \succeq 0$, $B, M \in Sym_n$, then $\langle B, M \rangle \ge 0$.

Proof: Since $B \in \text{Sym}_n$ it can be diagonalized by an orthogonal matrix $O, B = O\Delta O^T$, where $\Delta = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$ and $\lambda_i > 0$ are the eigenvalues of the positive definite matrix B. It is

$$\langle B, M \rangle = \operatorname{tr}(BM) = \operatorname{tr}(O\Delta O^T M) = \operatorname{tr}(\Delta O^T M O) = \operatorname{tr}(\Delta \tilde{M}) = \sum_{i=1}^n \lambda_i \tilde{m}_{ii} ,$$

where $\tilde{M} = O^T M O$ and \tilde{m}_{ii} are its diagonal elements. But $\tilde{M}^T = \tilde{M}$ and $x^T \tilde{M}x = (Ox)^T M Ox \ge 0$ for every $x \in \Re^n$, since $M \succeq 0$. So, it is also $\tilde{M} \succeq 0$ and thus $\tilde{m}_{ii} \ge 0$. Since, additionally, $\lambda_i > 0$, we conclude that $\langle B, M \rangle = \sum_{i=1}^n \lambda_i \tilde{m}_{ii} \ge 0$.

Theorem 2 If $A + A^T \prec 0$ then the semidefinite program defined in Theorem 1 has an optimal solution.

Proof: First we show that the set S of all matrices $M \succeq 0$ satisfying the equality constraints $\langle A_i, M \rangle = -p_i(0), i = 1, 2, ..., n - 1$, is non-empty. Indeed, the matrix

$$M = \operatorname{diag}(-p_1(0)/2a_{11}, -p_2(0)/2a_{22}, \dots, -p_n(0)/2a_{nn})$$

satisfies these conditions and, additionally, it is $M \succeq 0$, since $p_i(0) \ge 0$ and $a_{ii} < 0$ $(A + A^T \prec 0)$. Note that S is closed and convex. Now consider the function $f: S \to \Re$ defined by $f(M) = \langle A_n, M \rangle$ and the matrix $B = -\sum_{i=1}^n A_i = -(A + A^T) \succ 0$. From Lemma 1 and for $M \in S$, we have

$$\langle B, M \rangle \ge 0 \Rightarrow \langle A_n, M \rangle \le -\sum_{i=1}^{n-1} \langle A_i, M \rangle = \sum_{i=1}^{n-1} p_i(0) < +\infty \Rightarrow f(M) < +\infty$$
.

Thus $\sup_{M \in S} f(M) < +\infty$ and since S is closed the supremum is achieved for a $M_0 \in S$, so it is actually a maximum. The existence of an optimal solution is established.

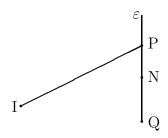


Figure 3: Construction of the reachable set of point I.

We finally show how the semidefinite programming formalism can be used for calculating the reachable set of point $I(p_1(0), p_2(0), \ldots, p_n(0))$. Consider the line ε parallel to p_n -axis, with $p_i = \text{constant} \ge 0$, $i = 1, 2, \ldots, n - 1$. The maximum achievable value of p_n on ε , starting from I, can be found by solving the following semidefinite program: Find $\max_M \langle A_n, M \rangle$ subject to $\langle A_i, M \rangle = p_i - p_i(0)$ for $i = 1, 2, \ldots, n - 1$ and $M \succeq 0$. If this program has a solution M_0 such that $p_n = p_n(0) + \langle A_n, M_0 \rangle \ge 0$, then let P be the point (p_1, p_2, \ldots, p_n) of ε , see Fig. 3. This point belongs to the reachable set of I. Additionally, every point $N(p_1, p_2, \ldots, p_{n-1}, p'_n)$ of ε with $0 \le p'_n \le p_n$, see Fig. 3, belongs also to the reachable set (first arrive at P and then use $m = (0, 0, \ldots, 1)^T$ to go down, since (10) gives $\dot{p}_n = a_{nn} < 0$, $\dot{p}_i = 0$ for $i \ne n$). Thus, the segment PQ, where $Q(p_1, p_2, \ldots, p_{n-1}, 0)$, is in the reachable set. By repeating the above procedure for all the allowed $\varepsilon \parallel p_n$, the reachable set of I can be constructed.

3 Remarks on the Rank of the Semidefinite Program Solutions

In the preceding section we saw that the bigger the rank of the optimal M for the semidefinite program, the more complicated is the optimal control law. Thus, it would be useful to know if there exist low rank optimal solutions and, additionally, rank upper bounds for them. Even more, we would like to know for what matrices A the corresponding semidefinite program has solutions of the lowest possible rank r = 1. In this section we present a series of results in these directions.

Lemma 2 Let us fix $A_1, A_2, ..., A_k \in Sym_n$ and $\alpha_1, \alpha_2, ..., \alpha_k \in \Re$. If there is a matrix $M \succeq 0$ such that

$$\langle A_i, M \rangle = \alpha_i, \quad i = 1, 2, \dots, k,$$

then there is a matrix $M_0 \succeq 0$ such that

$$\langle A_i, M_0 \rangle = \alpha_i, \quad i = 1, 2, \dots, k$$

and, additionally,

$$rankM_0 \le \left\lfloor \frac{\sqrt{8k+1}-1}{2} \right\rfloor$$
,

where $\lfloor \cdot \rfloor$ denotes the integer part of the embraced number.

Proof: See [2], chapter *II*, proposition 13.1.

Proposition 1 If $A + A^T \prec 0$ then there is an optimal solution M_0 to the semidefinite program defined in Theorem 1, with

$$rankM_0 \le \left\lfloor \frac{\sqrt{8n+1}-1}{2} \right\rfloor$$

Proof: From Theorem 2 we have that, since $A + A^T \prec 0$, the semidefinite program has an optimal solution $M \succeq 0$, which satisfies

$$\langle A_i, M \rangle = -p_i(0), \quad i = 1, 2, \dots, n-1, \quad \langle A_n, M \rangle = \mathcal{E}.$$

According to Lemma 2, there exists a $M_0 \succeq 0$ such that

$$\langle A_i, M_0 \rangle = -p_i(0), \quad i = 1, 2, \dots, n-1, \quad \langle A_n, M_0 \rangle = \mathcal{E}$$

and

$$\operatorname{rank} M_0 \le \left\lfloor \frac{\sqrt{8n+1}-1}{2} \right\rfloor$$

Obviously M_0 is also an optimal solution.

Corollary 1 If $A + A^T \prec 0$ and A is 2×2 , then the semidefinite program has an optimal solution of rank $r \leq 1$.

Proof: Apply Proposition 1 for n = 2. In general, the bound imposed by Lemma 2 is the best possible. However, there is one special case where it can be sharpened.

Lemma 3 For some positive integer r, let us fix k = (r+2)(r+1)/2 matrices $A_1, A_2, ..., A_k \in Sym_n$, where $n \ge r+2$, and k numbers $\alpha_1, \alpha_2, ..., \alpha_k \in \Re$. If there is a matrix $M \succeq 0$ such that

$$\langle A_i, M \rangle = \alpha_i, \quad i = 1, 2, \dots, k$$

and the set of all such matrices is bounded, then there is a matrix $M_0 \succeq 0$ such that

$$\langle A_i, M_0 \rangle = \alpha_i, \quad i = 1, 2, \dots, k$$

and, additionally,

 $rankM_0 \leq r$.

Proof: See [2], chapter *II*, proposition 13.4.

Proposition 2 If $A + A^T \prec 0$ and A is 3×3 , then the semidefinite program has an optimal solution of rank $r \leq 1$.

Proof: Since $A + A^T \prec 0$, the semidefinite program has an optimal solution $M \succeq 0$, which satisfies

$$\langle A_i, M \rangle = -p_i(0), \quad i = 1, 2, \quad \langle A_n, M \rangle = \mathcal{E}$$

From Lemma 3 we see that the choice r = 1 gives k = 3 = n, since n = 3 according to the hypothesis of the proposition. In order to apply Lemma 3, we just need to show that the set of optimal matrices, i.e. all the matrices $M \succeq 0$ satisfying the above relations, is bounded. Consider the matrix $B = -\sum_{i=1}^{3} A_i = -(A + A^T) \succ 0$. For a matrix $M \succeq 0$ in the set of optimal solutions, we have

$$\langle B, M \rangle = p_1(0) + p_2(0) - \mathcal{E} < +\infty$$
.

But from Lemma 1, we have also $\langle B, M \rangle = \sum_{i=1}^{3} \lambda_i \tilde{m}_{ii}$, where λ_i are the eigenvalues of B and \tilde{m}_{ii} the diagonal elements of the matrix $\tilde{M} = O^T M O$, O the orthogonal matrix diagonalizing B. Combining these we find that

$$\sum_{i=1}^{3} \lambda_i \tilde{m}_{ii} < +\infty$$

Since $\lambda_i > 0$ and $\tilde{m}_{ii} \ge 0$, the above relation implies that

$$\tilde{m}_{ii} < +\infty$$

thus

$$\operatorname{tr}(M) = \operatorname{tr}(M) < +\infty .$$

But

$$\langle M, M \rangle = \operatorname{tr}(M^2) \le (\operatorname{tr}(M))^2 < +\infty$$
,

since $M \succeq 0$. So indeed the set of optimal M is bounded and we can apply Lemma 3 with r = 1. This means that there is an optimal $M_0 \succeq 0$ with rank $M_0 \le 1$. Note that the bound that Proposition 1 gives in this case is only $\lfloor (\sqrt{8 \cdot 3 + 1} - 1)/2 \rfloor = 2$.

Lemma 4 Let us call an $n \times n$ matrix $A = \{a_{ij}\}$ r-diagonal if $a_{ij} = 0$ unless |i - j| < r. Suppose that the matrices $A_1, A_2, ..., A_k \in Sym_n$ are r-diagonal and there exists a matrix $M \succeq 0$ such that

$$\langle A_i, M \rangle = \alpha_i \in \Re, \quad i = 1, 2, \dots, k.$$

Then there exists a matrix $M_0 \succeq 0$ such that

$$\langle A_i, M_0 \rangle = \alpha_i, \quad i = 1, 2, \dots, k$$

and, additionally,

 $rankM_0 \leq r$.

Proof: See [2], chapter IV, corollary 10.3, problem 3.

Proposition 3 If $A + A^T \prec 0$ and A is r-diagonal, then the semidefinite program has an optimal solution of rank $\leq r$.

Proof: Since $A + A^T \prec 0$, there exists an optimal solution of the semidefinite program. Since A is r-diagonal, the corresponding A_i are also r-diagonal. Thus, we can apply Lemma 4, which assures the existence of an optimal solution of rank $\leq r$.

We conclude this section by noting that there is strong numerical evidence that the following conjecture is true.

Conjecture 1 If $A + A^T \prec 0$ then the semidefinite program has an optimal solution of rank r = 1.

4 Examples

In this section we solve problems 2 and 3 for some specific systems. We start from the system with

$$A = \begin{bmatrix} -\xi & -1 \\ 1 & -\xi \end{bmatrix}, \ \xi > 0 \ ,$$

which corresponds to system (3) appeared in the introduction. It is not necessary to solve numerically the corresponding semidefinite program, because we can attack this particular case analytically. Since $A+A^T = \text{diag}(-2\xi, -2\xi) \prec$ 0 and A is 2×2 , from Corollary 1 we have that there is an optimal solution to the semidefinite program with rank $r \leq 1$. Thus, there is an optimal constant vector $m = (m_1, m_2)^T$, solution to Problem 3. The system equation (10) with A given above and m constant gives

$$p_1(T_f) = p_1(0) - (\xi m_1^2 + m_1 m_2)T_f, \quad p_2(T_f) = p_2(0) + (m_2 m_1 - \xi m_2^2)T_f.$$
 (15)

Optimality requires

$$p_1(T_f) = 0 \Rightarrow T_f = \frac{p_1(0)}{\xi m_1^2 + m_1 m_2},$$
 (16)

 \mathbf{SO}

$$p_2(T_f) = p_2(0) + \frac{m_2 m_1 - \xi m_2^2}{\xi m_1^2 + m_1 m_2} p_1(0) .$$
(17)

In order to maximize $p_2(T_f)$, we just need to maximize the coefficient of $p_1(0)$. If we set $m_2/m_1 = x$, then this coefficient takes the form

$$f(x) = \frac{x - \xi x^2}{x + \xi} \,. \tag{18}$$

Before maximizing f, we find the allowed values of variable x. It should be $p_2(T_f) \ge p_2(0) \Rightarrow x - \xi x^2 \ge 0$ and $p_1(T_f) \le p_1(0) \Rightarrow x + \xi \ge 0$. These are both satisfied when $x \in [0, 1/\xi]$. We calculate the maximum of f in this interval. It is not difficult to verify that

$$f'(x) = -\frac{\xi(x^2 + 2\xi x - 1)}{(x + \xi)^2}$$
(19)

becomes zero at the point

$$x_0 = \sqrt{1 + \xi^2} - \xi \tag{20}$$

of the interval $[0, 1/\xi]$. Also verify that f'(x) > 0 for $x \in [0, x_0)$ and f'(x) < 0 for $x \in (x_0, 1/\xi]$. So $f(x_0)$ is a maximum in the interval $[0, 1/\xi]$. After some manipulation we find that

$$f(x_0) = x_0^2 . (21)$$

The maximum achievable value of p_2 is

$$p_2(T_f) = p_2(0) + x_0^2 p_1(0)$$
(22)

and the optimal unit vector is

$$m = \left(\frac{1}{\sqrt{1+x_0^2}}, \frac{x_0}{\sqrt{1+x_0^2}}\right).$$
(23)

The optimal trajectory in *p*-space is a straight line joining the points $(p_1(0), p_2(0))$ and $(0, p_2(T_f))$.

The maximum achievable value of r_2 is

$$r_2(\infty) = \sqrt{r_2^2(0) + x_0^2 r_1^2(0)} .$$
(24)

If the starting state is the point $(r_1(0), r_2(0)) = (1, 0)$, the maximum transfer efficiency takes the value

$$r_2(\infty) = x_0 = \sqrt{1 + \xi^2} - \xi$$
 (25)

For $\xi = 1$ this efficiency is $\sqrt{2} - 1$. The optimal controls u_1, u_2 for system (3), can be found by using the method described in section 2. If we define

$$\mathcal{M} = \max\left(1, \frac{x_0 r_1}{r_2}\right) \;,$$

the optimal policy can be realized as

$$u_1 = \frac{1}{\mathcal{M}}, \qquad u_2 = \frac{x_0 r_1}{r_2} u_1.$$

Observe that the initial point (1,0) is a stationary point of the optimal control policy $[r_2(0) = 0 \Rightarrow \mathcal{M} = \infty \Rightarrow u_1 = 0 \Rightarrow u_2 = 0]$. This optimal policy in the infinite horizon case should then be interpreted as the limit of optimal control policy for the corresponding finite time problem [Finite time for the r_i system, don't confuse it with the finite time problem for p_i which corresponds to the infinite horizon problem for r_i . It is the special case $k_1 = k_2 = 0$ of the finite time problem solved in the preceding chapter. The solution for this particular case can be found in [1]]. In practice, we give a small but finite value in $r_2(0)$ (an initial 'kick' from zero) which makes the optimal control law applicable. In Fig. 4(a) we plot the optimal controls u_1 and u_2 . In Fig. 4(b) we depict $r_1(t), r_2(t)$ and in Fig. 4(c) the corresponding optimal trajectory in r-space. For all these figures it is $\xi = 1$ and $(r_1(0), r_2(0)) = (1, 0)$.

Remark 1 The closure of the reachable set of point (1,0) is

$$\overline{\mathbf{R}((1,0))} = \{r_1, r_2 \ge 0 \mid \sqrt{r_2^2 + x_0^2 r_1^2} \le x_0\} ,$$

where $x_0 = \sqrt{1+\xi^2} - \xi$. This set is depicted in Fig. 4(c) for $\xi = 1$. The closure of the reachable set $\overline{\mathbf{R}((1,0,0,0))}$ for the corresponding bilinear system (1) is

$$\{(x_1, x_2, y_1, y_2) \in \Re^4 \mid \sqrt{(x_2^2 + y_2^2) + x_0^2(x_1^2 + y_1^2)} \le x_0\}.$$

The next case that we examine is the system with

$$A = \left[\begin{array}{rrr} -\xi & -1 & 0 \\ 1 & -\xi & -1 \\ 0 & 1 & -\xi \end{array} \right], \ \xi > 0$$

Since $A + A^T = \text{diag}(-2\xi, -2\xi, -2\xi) \prec 0$ and A is 3×3 , from Proposition 2 we have that the semidefinite program has a solution of rank $r \leq 1$. Now

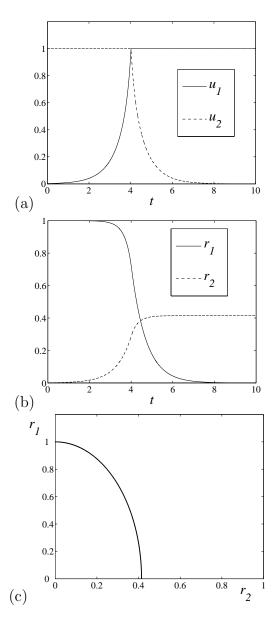


Figure 4: (a) Optimal controls $u_1(t)$ and $u_2(t)$ for system (3) when $\xi = 1$ and $(r_1(0), r_2(0)) = (1, 0)$ (b) The corresponding state variables $r_1(t)$ and $r_2(t)$ (c) The optimal trajectory in *r*-space.

let us become more specific, so set $\xi = 1$ and consider the starting point $(p_1(0), p_2(0), p_3(0)) = (1, 1, 0)$. The corresponding matrices A_i are

$$A_1 = \begin{bmatrix} -2 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & -2 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \quad A_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -2 \end{bmatrix}.$$

If we solve numerically the corresponding semidefinite program using some appropriate software package, for example SDPT3 [3], we find that the optimal matrix $M \succeq 0$ is

$$M = \begin{bmatrix} 0.1775 & 0.3225 & 0.1304 \\ 0.3225 & 0.5856 & 0.2368 \\ 0.1304 & 0.2368 & 0.0958 \end{bmatrix},$$

and the maximum achievable value of p_3 is

$$p_3(T_f) = p_3(0) + \langle A_3, M \rangle = \langle A_3, M \rangle = 0.2821$$
.

It is easy to verify that this matrix has two zero eigenvalues and one nonzero, so its rank is indeed r = 1. It can be written in the form $M = \lambda m m^T$, where $\lambda = 0.8589 (= T_f)$ is the nonzero eigenvalue and

$$m = (m_1, m_2, m_3)^T = (0.4546, 0.8257, 0.3339)^T$$

the corresponding eigenvector. This unit vector is the optimal solution for Problem 3.

The maximum achievable value of r_3 is $r_3(\infty) = \sqrt{p_3(T_f)} = 0.5311$. We find the optimal u_1, u_2, u_3 . Let us set

$$x_0 = \frac{m_2}{m_1} = 1.8163, \quad y_0 = \frac{m_3}{m_1} = 0.7345.$$

If we define

$$\mathcal{M} = \max(1, \frac{x_0 r_1}{r_2}, \frac{y_0 r_1}{r_3}) ,$$

then the optimal policy can be realized as

$$u_1 = \frac{1}{\mathcal{M}}, \quad u_2 = \frac{x_0 r_1}{r_2} u_1, \quad u_3 = \frac{y_0 r_1}{r_3} u_1.$$

Observe that the initial point (1,1,0) is a stationary point of the optimal control policy $[r_3(0) = 0 \Rightarrow \mathcal{M} = \infty \Rightarrow u_1 = 0 \Rightarrow u_2 = u_3 = 0]$. The situation is similar with that in the previous example. Again, the optimal policy in the infinite horizon case should be interpreted as the limit of the

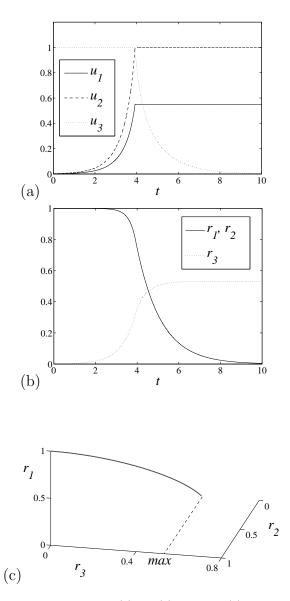


Figure 5: (a) Optimal controls $u_1(t), u_2(t)$ and $u_3(t)$ for system (5), with A the 3 × 3 matrix given in the text, when $\xi = 1$ and $(r_1(0), r_2(0), r_3(0)) =$ (1, 1, 0) (b) The corresponding state variables $r_1(t), r_2(t)$ and $r_3(t)$. Observe that $r_2(t)/r_1(t) = 1$ throughout. Remember that the optimal trajectory in p-space is a straight line ending at the point $(0, 0, p_3(T_f))$, so $p_2(t)/p_1(t) =$ $p_2(0)/p_1(0) = 1$ for the starting point (1, 1, 0) (c) The optimal trajectory in r-space.

optimal policy for the corresponding finite time problem. In practice, a small but finite value is given to $r_3(0)$. In Fig. 5(a) we plot the optimal controls u_1, u_2 and u_3 . In Fig. 5(b) we depict $r_1(t), r_2(t), r_3(t)$ and in Fig. 5(c) the corresponding optimal trajectory in r-space.

Another interesting case to examine is the same system with $\xi > 0$ unspecified and starting point $(p_1(0), 0, p_3(0))$. This problem can be solved analytically and has the practical application that it gives an upper bound for our ability to coherently control a specific dissipative quantum system [4]. As before, we know that there is an optimal constant vector $m = (m_1, m_2, m_3)^T$. From equations (10) we find

$$p_1(T_f) = p_1(0) - (\xi m_1^2 + m_1 m_2) T_f ,$$

$$p_2(T_f) = p_2(0) + (m_2 m_1 - \xi m_2^2 - m_2 m_3) T_f ,$$

$$p_3(T_f) = p_3(0) + (m_3 m_2 - \xi m_3^2) T_f .$$
(26)

Optimality requires

$$p_1(T_f) = 0 \Rightarrow T_f = \frac{p_1(0)}{\xi m_1^2 + m_1 m_2}$$
 (27)

and

$$p_2(T_f) = 0 \Rightarrow m_2 m_1 - \xi m_2^2 - m_2 m_3 = 0$$
. (28)

So, we have to maximize

$$p_3(T_f) = p_3(0) + \frac{m_3 m_2 - \xi m_3^2}{\xi m_1^2 + m_1 m_2} p_1(0)$$
(29)

subject to the constraint (28). We just need to maximize the coefficient of $p_1(0)$ under the same condition. If we set

$$\frac{m_2}{m_1} = x , \quad \frac{m_3}{m_1} = y ,$$

then this coefficient takes the form

$$g(x,y) = \frac{xy - \xi y^2}{x + \xi} , \qquad (30)$$

while the condition becomes

$$x(1 - \xi x - y) = 0 \Rightarrow y = 1 - \xi x .$$
(31)

Note that x=0 gives $g \leq 0$ so it is rejected. Using (31), g becomes a function of x only

$$f(x) = g(x, y(x)) = \frac{-\xi(1+\xi^2)x^2 + (1+2\xi^2)x - \xi}{x+\xi} .$$
(32)

We find the allowed values of x. A natural requirement is $p_3(T_f) \ge p_3(0) \Rightarrow y(x - \xi y) \ge 0 \Rightarrow (y \ge 0 \text{ and } x - \xi y \ge 0)$ or $(y \le 0 \text{ and } x - \xi y \le 0)$. Using (31) we find that the first option implies $x_1 \le x \le x_2$ and the second $x_2 \le x \le x_1$, where $x_1 = \xi/(1 + \xi^2), x_2 = 1/\xi$. Since $x_1 < x_2$, only the first option is acceptable, so it must be $x \in [x_1, x_2]$. For such x, the similar requirement $p_1(T_f) \le p_1(0) \Rightarrow x + \xi \ge 0$ is satisfied. So we maximize f in the interval $[x_1, x_2] = [\xi/(1 + \xi^2), 1/\xi]$. Solving the equation $f'(x_0) = 0$, we find

$$x_0 = \sqrt{\xi^2 + 2 - \xi}.$$
 (33)

Indeed, $x_0 \in [x_1, x_2]$. The corresponding maximum value of f is

$$f_{max} = \frac{x_0^4}{4} \ . \tag{34}$$

The maximum achievable value of p_3 is

$$p_3(T_f) = p_3(0) + f_{max}p_1(0) . (35)$$

Condition (28) implies that in the optimal case it is $\dot{p}_2 = 0$, so it is also $\dot{r}_2 = 0$. If $r_2(0) = 0$ then $r_2(t) = 0$ and, as we can see from (5), there is no transfer from r_1 to r_3 . What we actually examine here is the limiting case $r_2(0) = \epsilon \to 0^+$, where ϵ is an arbitrarily small positive number. We can still use condition (28), i.e. $\dot{r}_2 = 0$. The transfer $r_1 \to r_3$ takes place through r_2 which is held to the small constant value $r_2 = \epsilon$. The maximum achievable value of r_3 , which corresponds to the limit $\epsilon \to 0^+$, is

$$r_3(\infty) = \sqrt{r_3^2(0) + f_{max}r_1^2(0)}.$$
(36)

If the starting state is the point $(1, \epsilon, 0)$, where $\epsilon \to 0^+$, the maximum efficiency is

$$r_3(\infty) = \sqrt{f_{max}} = \frac{x_0^2}{2} = \frac{(\sqrt{\xi^2 + 2} - \xi)^2}{2}.$$
 (37)

For $\xi = 1$ we find that this efficiency is $2 - \sqrt{3}$. In Fig. 6 we plot the optimal controls $u_1(t), u_2(t), u_3(t)$, the state variables $r_1(t), r_2(t), r_3(t)$ and the optimal trajectory in r-space. Observe that the starting point is actually $(1, \epsilon, \epsilon)$. It is necessary to give a small positive initial value to r_3 , since the point $(1, \epsilon, 0)$ is still a stationary point of the optimal policy. If the starting point is $(1, \epsilon, \epsilon)$, then by solving the corresponding semidefinite program we find numerically the same efficiency as in (37), in the limit $\epsilon \to 0^+$.

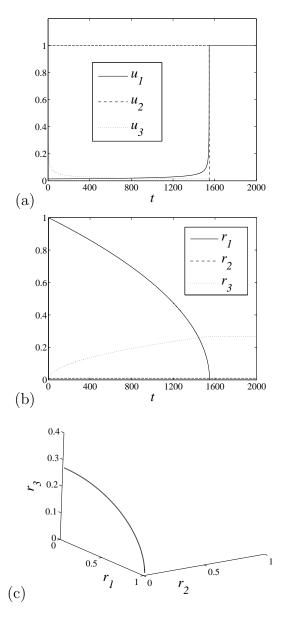


Figure 6: (a) Optimal controls $u_1(t), u_2(t)$ and $u_3(t)$ for system (5), with A the 3×3 matrix given in the text, when $\xi = 1$ and $(r_1(0), r_2(0), r_3(0)) = (1, \epsilon, \epsilon), 0 < \epsilon \ll 1$. Here we take $\epsilon = 0.01$ for convenience (b) The corresponding state variables $r_1(t), r_2(t)$ and $r_3(t)$. Note that transfer $r_1 \to r_3$ takes place through r_2 which is held to the small constant value $r_2 = \epsilon$. Thus, this transfer requires more time compared to the preceding examples (c) The optimal trajectory in r-space.

5 Conclusion

In this paper we studied a class of bilinear control systems, motivated by optimal control problems arising in the context of dissipative quantum dynamics. It was shown that the optimal solution and the reachable set of these systems can be found by solving a semidefinite program. As a practical result, solutions to these problems give upper bounds for the ability to coherently control quantum mechanical phenomena in presence of dissipation. In the area of coherent spectroscopy, these results translate into the maximum signal that can be obtained in an experiment. The paper also motivates the use of semidefinite programming to study reachable sets of more general bilinear control systems.

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