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Dynamic programming and viscosity solutions for the optimal control of quantum spin systems

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ABSTRACT

The purpose of this paper is to describe the application of the notion of viscosity solutions to solve the Hamilton–Jacobi–Bellman (HJB) equation associated with an important class of optimal control problems for quantum spin systems. The HJB equation that arises in the control problems of interest is a first-order nonlinear partial differential equation defined on a Lie group. Hence we employ recent extensions of the theory of viscosity solutions to Riemannian manifolds in order to interpret possibly non-differentiable solutions to this equation. Results from differential topology on the triangulation of manifolds are then used develop a finite difference approximation method for numerically computing the solution to such problems. The convergence of these approximations is proven using viscosity solution methods. In order to illustrate the techniques developed, these methods are applied to an example problem.

1. Introduction

Recently, there has been considerable attention directed at the problem of obtaining time optimal trajectories for open loop control of quantum spin systems [1–4]. These problems arise from applications which include NMR spectroscopy (to produce a time optimal trajectory), and the optimal construction of quantum circuits [5,6] (to minimize the number of logic gates required to construct a desired unitary transformation). These spin systems have the mathematical structure of a bilinear right invariant system on the special unitary group. Owing to the importance of the applications, there have been various approaches to solving these problems which utilize Lie theoretic arguments [2,7], calculus of variations [4,8], and dynamic programming [9,10].

In the dynamic programming approach, under appropriate regularity assumptions, the optimal cost function (value function) is the solution to a Hamilton–Jacobi–Bellmann (HJB) equation [11–13]. For many problems of interest this value function can be demonstrated to be non-differentiable. Hence there is the need for a more general notion of a solution to such partial differential equations (PDEs). A popular and successful concept of such a weak solution of nonlinear PDEs is the well-studied theory of viscosity solutions [14,15] on Euclidean spaces. Because the quantum spin problem leads to an HJB equation defined on a Lie group, we use extensions of viscosity solution theory to Riemannian manifolds [16–18] in order to interpret the solutions of this equation. For a detailed introduction to this topic, we refer the reader to [14,19] and the references contained therein.

In this article, we build up the components required for a rigorous application of viscosity solution theory on manifolds for quantum systems. This commences with an explanation of a discretization method based on the triangulation of manifolds [20] to solve the HJB equation for the optimal spin control problem. We then use viscosity solution concepts to prove the convergence of the solution obtained by this triangulation-based discretization scheme to the solution of the original HJB equation.

The structure of this article is as follows. We begin by describing the quantum spin control problem in Section 2. This is followed in Section 3 by a study of the regularity properties of the value function which play an important role in the solution of the associated HJB equation. After motivating the need for more generalized solutions of the HJB equation using an example system with a non-differentiable value function, we explain the use of the notion of viscosity solutions on Lie groups in Section 4. Results pertinent to the existence and uniqueness of such solutions are recalled from relevant literature and are modified to the framework of the problems introduced. In order to solve these optimal control problems numerically, we make use of the notion of triangulation of the group on which the system evolves. This concept and the proofs of convergence of the approximations to the actual solution using viscosity solution notions are introduced

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and developed in Section 5. In Section 6, the ideas developed are then applied to solve an example control problem on $SU(2)$ for which sample optimal trajectories and the value functions from the simulations are obtained. We conclude with comments and possible extensions in Section 7.

2. Problem description

2.1. System description

In this section, we introduce a mathematical model arising in applications of the open loop control of quantum systems. Given a compact connected matrix Lie group $\mathbf{G} = SU(2^n)$ with an associated Lie algebra $\mathfrak{g} = \mathfrak{su}(2^n)$ and smooth, right invariant vector fields $X_1, \dots, X_m$ in $\mathfrak{g}$, let the evolution of the system be given by

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \left\{ \sum_{k=1}^{m} v_k(t) X_k \right\} U, \qquad U(0) = U_0, \quad U, U_0 \in \mathbf{G}. \tag{1}$$

Here, $X_1, \dots, X_m$ are termed control vector fields. The v_i are elements of the control signal v which belongs to the class of piecewise continuous functions $\mathcal{V}$ with their range belonging to a compact subset $\mathbf{V}$ of the real m-dimensional Euclidian space $\mathbb{R}^m$, containing the origin. Without loss of generality, we may consider $\mathbf{V}$ to be the unit hypercube in $\mathbb{R}^m$ around the origin. We assume that the Lie algebra generated by the set $\{X_1, \dots, X_m\}$, using repeated Lie bracketing operations of all orders, is $\mathfrak{g}$. We denote the right-hand side of Eq. (1) above by $f(U, v)$. Given a control signal v and an initial point U_0, the solution to Eq. (1) at time t is denoted by $U(t; v, U_0)$. We denote by $\mathcal{T}$ a compact set in $\mathbf{G}$ with smooth closed boundary $\partial\mathcal{T}$. This set is the target set that we wish the system to reach.

Now, the following properties are satisfied at every point $x \in \mathbf{G}$:

- the system dynamics $f(\cdot)$ is driftless,
- if $\mathcal{X} := f(x, u)$ can be generated by a certain control $u \in \mathbf{V}$, then $-\mathcal{X}$ can also be generated using another element of the control set (in this case it would be $-u$),
- the dimension of the vector space at x, generated by the set of vector fields after all possible bracketing operations, has dimension equal to that of the group.

Hence we have from [21, Prop. 3.15] that the time to get from any point on the group to the identity element is bounded. Thus the entire group is reachable from the identity, and hence the problems dealt with in the next section are well defined.

2.2. Problem formulation

A large class of problems in the control of quantum spin systems and quantum circuit synthesis can be recast in terms of an optimal control problem with the following value function (optimal cost function):

$$S(U_0) = \inf_{v \in \mathcal{V}} \left\{ \int_0^{t_{U_0}(v)} \ell(U(s; v, U_0), v(s)) \mathrm{e}^{-\lambda s} \mathrm{d}s \right\}, \tag{2}$$

where $\ell : \mathbf{G} \times \mathbf{V} \to \mathbb{R}$ is continuous and $\lambda > 0$ is a real valued discount factor. Here, $t_{U_0}(v)$ denotes the time to reach the set $\partial\mathcal{T}$ starting from U_0 using control v. Note that, under the assumption that the cost $\ell(.)$ has a lower bound which is positive, we can then assume without loss of generality that the minimum of ℓ over $\mathbf{G} \times \mathbf{V}$ is 1. We now proceed to study some properties of the value function defined above.

3. Regularity of the value function

We begin by introducing certain quantities which will be used in the study of the regularity properties of the value function. Define the minimum time function

$$T(U) := \inf_{v \in \mathcal{V}} \{t_U(v)\}, \quad U \in \mathbf{G}, \tag{3}$$

which is the infimum of the time taken to reach the target set from a starting point U. The set of points, termed the reachable set, from which the desired target set may be reached in time τ is defined as

$$R(\tau) := \{U \in \mathbf{G} \mid T(U) < \tau\}.$$

A system is said to be *small time controllable* on a set $\mathcal{T}$ (denoted by STC $\mathcal{T}$) if

$$\mathcal{T} \subseteq \mathrm{int}(R(t)), \quad \forall t > 0. \tag{4}$$

Note that the assumption of small time controllability to the target set is required to obtain some of the results in this section, and it holds for the examples studied in this paper (and may be verified for any system under consideration).

We now introduce some results on the regularity of the value function whose proofs proceed along the lines of the arguments used in [14], with suitable modifications due to the Lie group setting.

Lemma 1. *[[14, Proposition 1.2 (Section 4)]] If the system is small time controllable on the set $\mathcal{T}$, then the value function is continuous in some open set containing the boundary $\partial\mathcal{T}$ of the set.*

Lemma 2. *Given a system evolving on a connected, compact Lie group, with dynamics (Eq. (1)) such that f, ℓ, and S satisfy the following conditions:*

1. *$f : \mathbf{G} \times \mathbf{V} \to T\mathbf{G}$ is continuous;*
2. *$\ell : \mathbf{G} \times \mathbf{V} \to \mathbb{R}$ is continuous;*
3. *S is continuous on some open set containing $\partial\mathcal{T}$;*

then S is bounded and continuous on $\mathbf{G}$.

Proof. This result consists of two cases of the value function.

- $\lambda = 0$: As indicated in Section 2.1, the time to get from any point on the group to the identity element is bounded. This, along with the bounds on ℓ, implies that the value function is bounded.
- $\lambda > 0$: In this case, the boundedness follows directly from the bounds on ℓ and the exponential decay factor $\lambda > 0$.

In both cases, the continuity proofs proceed along the lines of [14, Prop. 3.3 (Section 4)], with suitable modifications for the Lie group setting.

Example 3 (*Property of Value Function*)**.** Consider the following system, defined on the special unitary group $\mathbf{G} = SU(2)$:

$$\dot{U} = [I_z + vI_x]\,U, \tag{5}$$
$$U(0) = U_0,$$

where $v : [0, \infty) \to (-\infty, \infty)$ is a piecewise continuous control signal. Here, I_x and I_z are given by

$$I_x = \frac{-j}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad I_z = \frac{-j}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

Note that, in Eq. (6), we follow the mathematicians' convention in which I_x and I_z are skew-Hermitian matrices which belong to the Lie algebra $\mathfrak{su}(2)$ of the group $SU(2)$. The cost function to reach