

# Curse-of-Dimensionality-Free Control Methods for the Optimal Synthesis of Quantum Circuits

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**Abstract**—In this article we introduce the use of a recently developed numerical method from optimal control theory to the gate synthesis problem. This technique helps avoid the curse-of-dimensionality (COD) in the spatial dimension inherent in mesh based numerical approaches to solving control problems which also arise in optimal gate synthesis. In the proposed algorithm there is a however a growth in the complexity, related to the cardinality of the discretized control set, which is managed via a pruning technique. Hence an exponential speed up in the solution to a large class of control problems on spin systems is obtained. The reduced complexity method is then applied to obtain the approximate solution to an example problem on  $SU(4)$ - a 15 dimensional system.

## I. INTRODUCTION

The area of control of quantum spin systems has seen considerable attention focussed on the problem of optimal control of bilinear systems on the Lie group  $SU(2^n)$  (denoted by  $\mathbf{G}$ ). Such systems arise naturally in applications to nuclear magnetic resonance spectroscopy, quantum circuit synthesis etc. Of special interest in quantum computing are the bounds on the number of one and two qubit gates (specific members of  $\mathbf{G}$ ) required to synthesize a desired unitary operation (a desired element of  $\mathbf{G}$ ). This number is termed the gate complexity of the unitary.

Associated with the gate complexity problem is an optimal control problem whose cost function scales polynomially with the number of qubits of the desired gate if and only if the gate can be synthesized efficiently [1]. This motivates the solving of a class of optimal control problems which, in essence, may be viewed as an optimal time/distance control problems for systems evolving on the Lie group  $SU(2^n)$ . Various approaches have been taken to solve the gate complexity problem. These include considering efficient quantum circuit design via finding a least path-length trajectory on a Riemannian manifold [1], or through the use of Pontryagin's maximum principle to obtain necessary conditions for the minimum time implementation of quantum algorithms [2]. Alternative techniques using Lie group decomposition methods to obtain the optimal sequence of gates to synthesize a unitary (for certain classes of systems) were developed in [3].

In [4] an application of the dynamic programming approach from optimal control to the control problem for gate complexity for very general cost functions was introduced.

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This technique offered sufficient conditions to find an optimal sequence of one and two qubit gates which implement a desired unitary, in principle, for any number of qubits. However dynamic programming suffers from the curse of dimensionality (COD) in the spatial dimension when a grid based numerical method is used to solve the problem. The complexity of such an approach grows as an exponential of the dimension ( $4^n - 1$ ) of the state space for a system of  $n$  qubits. Hence it is intractable to solve the gate complexity problem on systems larger than single qubits using such grid based methods.

Recently there have been methods developed for a curse-of-dimensionality-free approach to solve certain classes of control problems on Euclidean space [6], [7] using the max-plus property of the semigroup operator corresponding to solution of the Hamilton-Jacobi-Bellman PDE. In this approach the problem is discretized in both time as well as in the control space, thus avoiding a growth in the spatial dimensions. There is a growth in the cardinality of the set of control sequence arising from this approach, which is managed by using a projection technique. The proposed method helps reduce the growth in dimensionality of the problem to an exponentially slower extent than in the mesh based methods thereby making the numerical study of larger systems possible.

We describe herein the application of the min-plus curse-of-dimensionality-free theory for a system of  $n$ -qubits and present simulation results for a 2-qubit gate synthesis example. Note that for this example a grid based solution method with an extremely conservative mesh of 20 points in each dimension with a total of 20 iterations over the space and an estimated time of 0.0001 seconds to propagate the value function via value iteration [4] at each point in the mesh would take  $1.8 \times 10^{13}$  hours to compute. On the other hand, with the numerical technique discussed herein, one can obtain a reasonable approximate solution in 7 hours on a standard desktop computer. For this class of problems, min-plus based numerical methods are many, many orders of magnitude faster than traditional schemes.

## II. MATHEMATICS SKETCH

We now briefly indicate the underlying mathematics. Previously [7], max-plus (and min-plus) methods were developed for a class of infinite time-horizon problems over all of  $\mathbb{R}^n$  (i.e., on the Euclidean space without state constraints). Further, the Hamiltonian was represented as a point-wise maximum (or minimum) of linear/quadratic forms.

The natural structure in which to frame the problem considered herein, is that of a minimum-time control problem for a system constrained to evolve on the Lie group  $\mathbf{G} = SU(2^n)$ . Although the concept remains the same, the entire underlying analysis is different from previous applications of the max (min) plus methods. First, we note that, due to symmetries the general form of the problem may be cast as that of finding the minimum time control strategy to drive the system from initial state,  $U_0 \in \mathbf{G}$ , to the identity,  $I$ . The system dynamics and initial condition are

$$\dot{U} = \left[ \sum_{m=1}^M \nu^m(t) H_m \right] U(t), \quad U(s) = U_0 \quad (1)$$

where  $\nu(t) = (\nu_1(t), \nu_2(t) \dots \nu_M(t)) \in \mathcal{N} \doteq \{\nu : [s, \infty) \rightarrow E\}$ . Here  $E = \{e^1, e^2 \dots e^M, 0\}$  and  $e^k$  is the  $M$  element vector with its  $k$ -th element set to 1 and the rest rest to 0. The next step is to convert the minimum-time formulation into a finite time-horizon payoff problem (for which the min-plus theory exists). This requires an upper bound on the minimum time required to drive the system to the identity. Such a bound is given by the following result:

*Theorem 2.1:* Given  $U_0 \in \mathbf{G}$ , there exists  $\bar{H} \in su(2^n)$  with  $\|\bar{H}\| = 1$  and  $T \in [0, \infty)$  such that  $U_0 = e^{\bar{H}T}$ . Moreover, there exists  $\delta_5 > 0$  such that for all  $U_0 \in \mathbf{G}$  the infimum time to drive the system from  $U_0$  to  $I$  is bounded above by

$$\tau = \begin{cases} \frac{4\sqrt{2}}{\sqrt{2}-1} \sqrt{T} + 2T & \text{if } T < \delta_5, \\ \frac{4\sqrt{2}}{\sqrt{2}-1} \frac{T}{\sqrt{\delta}} + 2T & \text{if } T \geq \delta_5, \end{cases} \\ \leq \begin{cases} \left[ \frac{4\sqrt{2}}{\sqrt{2}-1} + 2 \right] \sqrt{T} & \text{if } T < \delta_5, \\ \left[ \frac{4\sqrt{2}}{\sqrt{2}-1} + 2 \right] \frac{T}{\sqrt{\delta}} & \text{if } T \geq \delta_5, \end{cases}$$

where in the case  $T \geq \delta_5$ , we let  $\bar{N} = \lceil (T/\delta_5) \rceil$  and  $\delta = T/\bar{N}$ .

Given the bound above, we can use a finite-time horizon payoff of the form

$$J(U_0; \nu, s) \doteq \int_s^T \chi(\nu(t)) dt + \frac{1}{\varepsilon} \phi(U(T)),$$

where  $\hat{\chi} : E \rightarrow \{0, 1\}$  is the characteristic function defined as  $\hat{\chi}(e) = 1$  if  $\|e\| = 1$  and  $\chi(e) = 0$  otherwise. We take

$$\phi(U) := \text{tr}[(U - I)^*(U - I)] = \text{tr}[2I - U - U^*]. \quad (2)$$

Here,  $\varepsilon$  is sufficiently small so that this problem is approximately equivalent to the minimum-time problem. The value function is

$$\hat{V}(U_0, s) = \inf_{\nu \in \mathcal{N}} J(U_0; \nu, s).$$

Equation (2) above can be rewritten as

$$\phi(U) = c_0 + P_0 \cdot U, \quad (3)$$

where

$$c_0 = 2n, \quad P_0(U) = -\text{tr}[U] - \text{tr}[U^\dagger], \quad (4)$$

encode the cost at the initial time when no control has been applied.

Using this formulation, and applying an induction argument we may convert the time-discretized backward dynamic program (over time-steps, each of duration  $\delta$ , indexed by  $\mathcal{K} \doteq \{0, 1, 2, \dots K\}$ ) into the form

$$V_k(\hat{U}) = \min_{\lambda_k \in \Lambda_k} \left[ c_{\lambda_k}^k + P_{\lambda_k}^k \cdot \hat{U} \right],$$

where  $\Lambda_k$  denotes the set of  $k$ -step control sequences. This set is generated from the  $(k - 1)$ -step control sequence via the operation  $\{1, 2, \dots M\} \times \Lambda_{k-1}$ . For all  $k$  there is a natural one-to-one, onto mapping between each  $k - 1$ -step control sequence  $\lambda_{k-1}$  and  $\lambda_k$  that can be denoted by  $\sigma_k : (m, \lambda_{k-1}) \mapsto \lambda_k$ . Note that the initial control set that performs no operation is  $\Lambda_0 = \{1\}$ . Using the notation described above, we have the following recursive relationship that generates the sequence of scalars  $c_{\lambda_k}^k$  and operators  $P_{\lambda_k}^k$

$$c_{\sigma_k(m, \lambda_{k-1})}^k = c_{\lambda_{k-1}}^{k-1} + \chi_m \delta \quad (5)$$

$$P_{\sigma_k(m, \lambda_{k-1})}^k = A_m^T P_{\lambda_{k-1}}^{k-1}. \quad (6)$$

Here  $A_m^T$  denotes the state transition matrix arising from the application of the control indexed by  $m$  in the set of controls  $\{1, 2, \dots M\}$  and  $\chi_m$  indicates the corresponding value of the  $\chi$  function applied to that choice of control. Thus there is a easily computable set of parameters generated by Eq. (6) which are obtained without any spatial discretization thereby avoiding the curse of dimensionality arising from the spatial dimensions.

However an important aspect of note is the growth in the complexity of the solution process, arising from the growth of the size of the control index set  $\Lambda_k$ . This must be attenuated and is carried out by projecting the representation,  $V_k$ , onto the optimal lower-dimensional min-plus vector space at each step via a pruning process. A method similar to that applied in [5] is employed where techniques from semi-definite programming [8] to help in the projection stage

### III. EXAMPLE

In this section we apply the theory developed thus far to an example of a 2-qubit system which is a particular case of the system dynamics in Eq (1) with  $m = 5$  and a control set given by  $\{I \otimes \sigma_x, I \otimes \sigma_z, \sigma_x \otimes I, \sigma_z \otimes I, \sigma_x \otimes \sigma_z\}$  i.e. a set of four 1-body terms and one 2-body term. Here

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

denote the standard Pauli matrices which are elements of the Lie algebra of  $su(2)$ . This control set is sufficient to generate the entire Lie algebra  $su(4)$ , thereby ensuring controllability.

To visualize the solution we use the fact that the Lie algebra  $su(2^n)$  is isomorphic to the Euclidean space and that every point on the Lie group  $SU(4)$  can be generated via the exponential map from the algebra. Hence the optimal cost function can be represented as a function on points in the Euclidean co-ordinates. Thus in order to plot the cost function on the group, we determine the point in the Lie algebra that corresponds to the point on the group at which the optimal cost function has been determined. We then

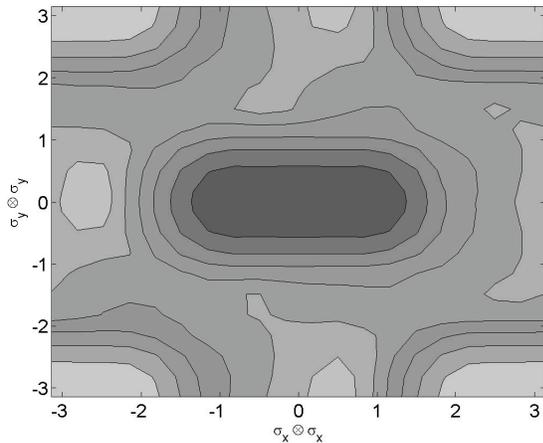


Fig. 1. Plot of the cost function in the plane  $\sigma_x \otimes \sigma_x$  vs  $\sigma_y \otimes \sigma_y$  with the cost ratio of available 1-body Hamiltonian to the 2 body Hamiltonian  $\sigma_x \otimes \sigma_x$  set to 1.

plot the cost function for 2-dimensional slices of interest in the algebra. We note that this mapping is surjective and hence there are multiple points in the algebra mapping to the same point on the group. Thus the figures obtained must be carefully interpreted.

Figure 1 indicates the approximate optimal cost function at points chosen in the plane of interest  $\sigma_x \otimes \sigma_x$  vs  $\sigma_y \otimes \sigma_y$ . Regions of darker shading indicate unitaries which are easier (lower cost) to generate while the lighter areas show gates which are costly to synthesize. Contour lines are used to connect points having the same cost function. As the generation of motion along the  $\sigma_y \otimes \sigma_y$  direction requires the use of Lie bracketing, which thereby causes a larger time to traverse along that direction. This is indicated by the oblong contours in the resulting figure.

#### IV. CONCLUSION

This article introduces some recent extensions of the min-plus method for a class of optimal control problems on quantum systems evolving on certain manifolds. The class of problems described herein is a novel addition in the literature to those considered thus far in the application of min-plus techniques to optimal control. In the technique described herein we exploited the preservation in structure of the optimal cost function to obtain substantial improvements in computational speed of numerical algorithms. Instead of the curse of dimensionality in the spatial dimension, we now have a much more manageable growth in dimensionality that depends on the number of elements in the discretization of the control set. An approximate solution to a previously intractable problem on a 15-dimensional system was obtained using the theory developed herein. We note that this is an approximate solution; the determination of various properties of these algorithms such as error bounds, rate of convergence, effect of different pruning methods etc. would be the subject for further research.

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