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PROJECT REPORT

Quantum Control via Discrete-Time Optimal Control

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Abstract

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This report describes the theoretical framework behind the discrete-time Pontryagin Maximum Principle and outlines a template for its potential application to qubit control. In experimental systems, qubit control is achieved by sending pulses that are discretized in time, a constraint rooted in the DAC-based signal generation equipment. Quasi-continuous assumptions underline every attempt at optimal control of qubits due to the finite rise time associated with DACs, and the desire for smooth, bandwidth-limited control pulses. Incorporating this discrete nature of control right at the synthesis stage is desirable for accurate system modelling and subsequent optimization. Often, there are particular frequencies which one would like to avoid to ensure precise control. The discrete-time Pontryagin Maximum Principle provides first-order conditions for optimality, naturally incorporates the discrete nature of the pulses, and is capable of handling experimental constraints even in the frequency domain. A simple problem formulation is presented, and various experimental constraints are considered on the dynamics of the system, the control pulses actuated and the bandwidth of operation. Shooting techniques to solve the resulting two-point boundary value problem are discussed and some techniques for practical implementation are ideated.

Acknowledgements

I am extremely grateful to my supervisor Debasish Chatterjee for his guidance, resourcefulness and patience throughout this project. Our very first meeting set the tone for how this dynamic would shape my ideal expectations not just from a guide, but from a serious research career. I recall sharing a few ideas I had regarding robust geometric quantum optimal control, requiring a nontrivial foundation in differential geometry and geometric control. My initial motivation for picking a project under Prof. Chatterjee was to leverage his substantial experience in these fields and explore new applications to quantum control.

During the first meeting, we sat down to discuss my ideas, he had pulled up several papers, earmarked relevant sections, found additional resources and arranged them on his desk in preparation for our discussion. Such enthusiasm, attention to detail and curiosity for new ideas simply lead by example. While the focus of this project has since shifted towards an extension of recent promising results from his research towards applications on quantum control, his mathematical rigour, patient explanations, immense resourcefulness and attention to detail stand out as exemplary qualities that I seek to emulate as I mature further as a researcher.

I would also like to thank Siddhartha Ganguly and Pradyumna Paruchuri for their helpful discussions and sharing comprehensive resources. Their papers have laid the foundation for this recent foray of mine, and have been a delight to read in such depth. Finally, I would like to thank my friends for their patience in entertaining a consistently occupied cog in their social network.

Contents

List of Abbreviations

OCT	**O**ptimal **C**ontrol **T**heory
PMP	**P**ontryagin **M**aximum **P**rinciple
HJB	**H**amilton-**J**acobi-**B**ellmann
GRAPE	**GR**adient **A**scent **P**ulse **E**ngineering
GOAT	**G**radient **O**ptimization (of) **A**nalytic con**T**rols
OCP	**O**ptimal **C**ontrol **P**roblem
NR	**N**ewton-**R**aphson
RM	**R**obbins-**M**onro
SA	**S**tochastic **A**pproximation
ODE	**O**rdinary **D**ifferential **E**quation
BVP	**B**oundary **V**alue **P**roblem
DAC	**D**igital (to) **A**nalog **C**onverter

1 Introduction

Quantum technology is an effort to find practical utility in devices based on the principles of quantum mechanics. This necessitates a precise manipulation of quantum devices using external electromagnetic fields (controls). Quantum control refers to methods that govern the time evolution of control parameters to perform specific manipulations of the quantum physical objects. This has wide-ranging applications in quantum computing, sensing and simulation.

Most quantum control protocols compute the control law in an open-loop configuration i.e., without experimental feedback. For such problems, optimal control theory (OCT) is a powerful tool that allows a prescribed process to be carried out while minimizing a cost (the cost could be experimental constraints like control time, power or bandwidth). A few key advantages of this approach are its flexibility concerning constraints and the optimal nature of pushing the driven dynamics to the physical limits. OCT can be understood as a generalization of the classical calculus of variations for dynamically constrained problems. The Pontryagin maximum principle (PMP) (Pontryagin, 1987) is a modern form of OCT developed by Pontryagin and his coworkers in the late 1950s. Recent tools from differential geometry have been applied to control theory, significantly increasing their ability to handle problems of growing complexity. A deep analogy can be carried out between OCT and finding the minima of a real function of several variables.

OCT was first applied to quantum processes in the context of physical chemistry to steer chemical reactions or to control spin dynamics in nuclear magnetic resonance. For quantum technologies, many recent results have been established in the past decades such as the minimum duration to generate high-fidelity quantum gates. The interested reader is directed to (Glaser et al., 2015; Mahesh, Batra, and Ram, 2022; Wilhelm et al., 2020) for excellent reviews of recent progress and an introduction to this exciting field. A rich zoo of quantum optimal control protocols has been developed that address various experimental needs, functional spaces of interest and robustness to diverse sources of noise.

In this chapter, we follow an excellent tutorial on using PMP for quantum optimal control (Boscain, Sigalotti, and Sugny, 2021) and will limit our focus to the optimal control of an open-loop finite-dimensional system using the PMP. We shall consider only analytical and geometric techniques to solve low-dimensional control problems. We stress however that there are

several distinctions to be drawn between problem classes: finite- or infinite-dimensional systems, open- or closed-loop control, linear or nonlinear dynamical systems, geometric or numerical optimal control, the PMP or Hamilton-Jacobi-Bellmann (HJB) approach, etc. We have only selected a narrow intersection of these problem classes to explore. To draw a connection with state-of-the-art applications of optimal control to quantum systems, we describe a link between the PMP and the now ubiquitous GRAPE algorithm (Khaneja et al., 2005), a gradient-based optimization algorithm for quantum control.

1.1 Two-level Quantum System

A general problem in quantum control is to prepare a given quantum state (target) using a specific time-dependent electromagnetic pulse (microwave pulses for the case of superconducting qubits). A naive control scheme uses Gaussian, cosine or flat-top pulse envelopes to control qubits in an agnostic one-size-fits-all approach. In an ideal system, the total power delivered to the system (area under the pulse) is the only factor governing the dynamical evolution. However, in realistic systems, the freedom to shape pulses can be exploited to intentionally mitigate exposure to errors in the dynamical evolution.

1.1.1 Driven control

Consider a control driving a two-level quantum system from the ground to the excited state (a π pulse). This system is described by a wave function $\psi(t)$ and its dynamics are governed by the Schrödinger equation

$$i\dot{\psi} = \begin{pmatrix} E_0 & \Omega(t) \\ \Omega^*(t) & E_1 \end{pmatrix} \psi,$$

where units such that $\hbar = 1$ have been chosen. E_0 and E_1 denote the energies of the ground and excited states respectively, while $\Omega(t)$ corresponds (to a multiplicative factor) to a complex external field whose real and imaginary parts are for example the in-phase (I) and quadrature (Q) of a microwave signal. We consider resonant signals such that the carrier frequency ω is equal to the energy difference $E_1 - E_0$, namely,

$$\Omega(t) = u(t)e^{i(E_1-E_0)t},$$

where the amplitude $u(t)$ represents the control and is assumed to be real.

Now, apply a time-dependent change of variables corresponding to the choice of a rotating frame. The time evolution of $\tilde{\psi} = \Upsilon^{-1}\psi$, with $\Upsilon = \mathrm{diag}(e^{-iE_0t}, e^{-iE_1t})$, satisfies the differential equation

$$i\dot{\tilde{\psi}} = \begin{pmatrix} 0 & u(t) \\ u(t) & 0 \end{pmatrix} \tilde{\psi}.$$

Let $c_1 = x_1 + iy_1$ and $c_2 = x_2 + iy_2$ be the two complex coordinates of $\tilde{\psi}$ in a basis of the Hilbert space $\mathbb{C}^2$, where the indices 1 and 2 respectively correspond to the ground and excited states. As ψ is a state of norm 1 and Y is a unitary operator, it can be deduced that $x_1^2 + y_1^2 + x_2^2 + y_2^2 = 1$. Starting from the state $x_1 = 1$, the goal of the control is to bring the system to a target satisfying $x_2^2 + y_2^2 = 1$. The Schrödinger equation is now equivalent to the following set of equations for the coefficients x_k and y_k:

$$\begin{aligned} \dot{x_1} &= uy_2, \quad \dot{y_1} = -ux_2, \\ \dot{x_2} &= uy_1, \quad \dot{y_2} = -ux_1. \end{aligned}$$

Since u is a real control, it can be noted that the first and last equations are coupled to each other, and decoupled from the two others. Alternatively, the initial state of the dynamics is only connected to states for which $y_1 = x_2 = 0$, i.e., such that $x_1^2 + y_2^2 = 1$. Thus, we see that our system evolves on a circle. For our control objective of driving a transition from the ground to the excited state, the relevant states correspond to $y_2 = \pm 1$. It can be verified trivially that such target states can be reached at least with a constant control u, no pulse shaping is necessary. In control theory, such a formulation of the control problem and analysis of the reachable set from the initial state is a necessary due diligence to be established before deriving a specific control procedure. This problem formulation will be elaborated upon in the following section.

1.1.2 Optimal control

The circular geometry of the dynamics helps us simplify the corresponding equations by introducing the angle θ such that $x_1 = \cos\theta$ and $y_2 = \sin\theta$, with $\theta(0) = 1$. We arrive at

$$\dot{\theta} = -u(t),$$

where the target state is here defined as $\theta_{\text{fi}} = \pm\pi/2$. Without loss of generality, we can use symmetry to fix $\theta_{\text{fi}} = -\pi/2$. Several control solutions u exist to reach this state and a specific protocol can be selected by choosing to simultaneously minimize a *cost function* of the state of the system and the control.

An example of the cost could be the control time. Let us consider the goal of the optimal control procedure to find the control u steering the system to the target state in minimum time (minimum cost). If we consider constant controls at first $u(t) = u_0$ with $u_o \in \mathbb{R}$. The duration of the process is trivially $T = \pi/2u_0$. and this solution reveals a key problem regarding the existence of a minimum in optimal control. Here, arbitrarily fast controls can be achieved by considering larger and larger amplitudes u_0 and an optimal trajectory minimizing the transfer time does not exist. It can be shown however, that an optimal solution does exist if the set of available controls is restricted to a bounded interval, e.g., $u(t) \in [-u_m, u_m]$, where u_m is the

maximum amplitude. In such a case, the optimal pulse is the control of the maximum amplitude, with the minimum time equal to $\pi/2u_m$.

For an illustration of solving an optimal control problem, let us consider the same transfer but in a given fixed time T, attempt to minimize the energy (power) associated with the control, i.e., the term $\int_0^T u(t)^2 dt/2$. We have no additional constraint on the control and enforce $u(t) \in \mathbb{R}$. The target state is reached if $\int_0^T u(t)dt = \pi/2$. Let us introduce the Lagrange multiplier $\lambda \in \mathbb{R}$, and transform this constrained optimization problem into the minimization of the functional

$$J = \int_0^T \left(\frac{u(t)^2}{2} + \lambda u(t) \right) dt - \lambda \frac{\pi}{2}.$$

Let us denote by H the function $H = -u^2/2 - \lambda u$, the Euler-Lagrange principle then leads to $\partial H/\partial u = 0$, i.e., $u(t) = -\lambda$. Using the constraint on the dynamics, we finally reach the optimal control $u(t) = \pi/2T$.

The optimal solution in such a simple example does not require the complete machinery of the Pontryagin maximum principle that follows below. However, this introduces the main tools used in the PMP - the Lagrange multiplier, the Pontryagin Hamiltonian H (often referred to as the pre-Hamiltonian later in this report to distinguish it from the quantum mechanical Hamiltonian), and the maximization condition $\partial H/\partial u = 0$.

A few comments on this example are necessary here. The dynamical constraint is quite simple as the dimension of the state space is the same as the number of controls (1), the dynamics can be exactly integrated, and the set of controls satisfying the constraint $\int_0^T u(t)dt = \pi/2$ is regular. However, this isn't the case for a general nonlinear control system for which (1) the Lagrange multipliers are not easily found, and can be time-dependent, and (2) abnormal Lagrange multipliers can appear if the set of controls satisfying the constraint is not regular. Further details are discussed in a later section on first-order conditions.

1.2 Formulation of the Control Problem

1.2.1 Dynamics

A finite-dimensional control system is a dynamical system governed by an equation of the form

$$\dot{q}(t) = f[q(t), u(t)], \tag{1.1}$$

where $q : I \to M$ represents the state of the system, I is an interval in $\mathbb{R}$, and M is a smooth manifold whose dimension is denoted by n. Recall that a manifold is a space that locally (but perhaps not globally) looks like $\mathbb{R}^n$.

Manifolds appear naturally in quantum control to describe, for instance, the $(2N-1)$-dimensional sphere S^{2N-1}, which is the set of the wave functions of a N-level quantum system (a ubiquitous example is the 3D Bloch sphere for a two-level quantum system).

The control law is $u : I \to U \subset \mathbb{R}^m$ and f is a smooth function such that $f(\cdot, \bar{u})$ is a vector field on M for every $\bar{u} \in U$. An example of a set U of possible values of $u(t)$ is given by $U = [-1, 1]^m$, meaning that the size of each of the coordinates of u is at most one. The set U can be the entire $\mathbb{R}^m$ if there is no control constraint.

To verify that Eq. 1.1 is well posed from a mathematical perspective, consider the case in which $I = [0, T]$ for some $T > 0$ and u belongs to a space of regular enough functions *mathcalU* called the class of *admissible controls*.

Piecewise continuous controls form a subset of admissible controls, and in experimental implementations of quantum control, they are the only control laws that can be reasonably applied. However, the class of piecewise constant controls is not suited to prove the existence of optimal controls (we shall later describe a discrete-time variant of the PMP that provides consideration for this very limitation).

For an admissible control $u(\cdot)$ and an initial condition $q(0) = q_{\text{in}} \in M$, there exists a unique solution $q(\cdot)$ of Eq. 1.1, defined at least for small times. A continuous curve $q(\cdot)$ for which there exists an admissible control $u(\cdot)$ such that Eq. 1.1 is satisfied is called an *admissible trajectory*.

Let us now discuss a typical situation encountered in quantum control. Consider the time evolution of the wave function of a closed N-level quantum system. In this case, under the dipolar approximation, the dynamics is governed by the Schrödinger equation (in units where $\hbar = 1$)

$$i\dot{\psi}(t) = \left(H_0 + \sum_{j=1}^{m} u_j(t) H_j \right) \psi(t), \tag{1.2}$$

where ψ, the *wave function*, belongs to the unit sphere in $\mathbb{C}^N$ and $H_0, \ldots, H_m$ are $N \times N$ Hermitian matrices. The control parameters $u_j(t) \in \mathbb{R}$ are the components of the control $u(\cdot)$. This control problem has the form of Eq. 1.1 with $n = 2N - 1$, $M = S^{2N-1} \subset \mathbb{C}^N$, $q = \psi$, and $f(\psi, u) = -i(H_0 + \sum_j^m u_j H_j)\psi$. Note that the uncontrolled part corresponding to the H_0 term is called the *drift*. The solution of the Schrödinger equation can also be expressed in terms of the unitary operator $\mathbf{U}(t, t_0)$, which connects the wave function at time t_0 to its value at t : $\psi(t) = \mathbf{U}(t, t_0)\psi(t_0)$. The *propagator* $\mathbf{U}(t, t_0)$ also satisfies the Schrödinger equation

$$i\dot{\mathbf{U}}(t, t_0) = \left(H_0 + \sum_{j=1}^{m} u_j(t) H_j \right) \mathbf{U}(t, t_0) \tag{1.3}$$

with initial condition $\mathbf{U}(t_0, t_0) = \mathbb{I}_N$. In quantum computing, the control problem is usually defined concerning the propagator $\mathbf{U}$. Eq. 1.3 has the form of Eq. 1.1 with $M = U(N) \subset \mathbb{C}^{N\times N}$ and $q = \mathbf{U}$.

We remark that the wave function formalism is well suited to describe pure states of isolated quantum systems, but when systems are imperfectly characterized the correct formalism to be used is that of mixed-state quantum systems using density matrices and Lindbladian dynamics for open quantum systems. We do not discuss this complication here.

1.2.2 Initial and final states

In most quantum control problems, the goal is not to bring the system from an initial state q_{in} to a final state q_{fi}, but rather to reach at time T a smooth *submanifold* $\mathcal{T}$ of M called the target:

$$q(0) = q_{\text{in}}, \quad q(T) \in \mathcal{T}. \tag{1.4}$$

This is the case in the population transfer from a state ψ_{in} to an eigenstate ψ_{fi} of the field-free (drift) Hamiltonian H_0. In this case, since the phase of the final state is not physically relevant, $\mathcal{T}$ is characterized by $\{e^{i\theta}\psi_{\text{fi}} \| \theta \in [0, 2\pi]\}$. It is also possible that the initial condition $q(0) = q_{\text{in}}$ is generalized to $q(0) \in \mathcal{S}$, where $\mathcal{S}$ is a smooth submanifold of M.

In the Bloch sphere picture of a two-level quantum system, this corresponds to all states with the same Z projection upon measurement being computationally equivalent. The changes necessary for this consideration are straightforward, so we concern ourselves simply with the precisely defined transition from an initial state q_{in} to a final state q_{fi}. Finally, it should be noted that the time T can be fixed or free, as is necessary for a time-minimum control problem.

1.2.3 Optimal control problem

We can use two optimal control approaches to steer the system from q_{in} to a target $\mathcal{T}$ in our optimal control problem (OCP).

- Approach A: prove that the target $\mathcal{T}$ is reachable from q_{in} (in time T if the final time is fixed or in any time otherwise) and then find the best possible control realizing the transfer. Essentially, we must show that

  $$\mathcal{T} \cap \mathcal{R}(q_{\text{in}}) \neq \emptyset \text{ if } T \text{ is free},$$

  where $\mathcal{R}(q_{\text{in}}) := \{\bar{q} \in M \mid \exists\, T$ and an admissible trajectory $q : [0, T] \to M$ such that $q(0) = q_{\text{in}}, q(T) = \bar{q}\}$ or that

  $$\mathcal{T} \cap \mathcal{R}^T(q_{\text{in}}) \neq \emptyset \text{ if } T \text{ is fixed},$$

where $\mathcal{R}^T(q_{\text{in}}) := \{\bar{q} \in M \mid \exists$ an admissible trajectory $q : [0, T] \to M$ such that $q(0) = q_{\text{in}} q(T) = \bar{q}\}$, and then solve the minimization problem

$$\int_0^T f^0[q(t), u(t)]dt \to \min, \tag{1.5}$$

where $f^0 : M \times U \to \mathbb{R}$ is a smooth function, which in most quantum control applications depends solely on the control. For example, the function representing energy used in a control process, $\int_0^T u^2(t)dt$. The control time T can be fixed or free. The integral is usually called the *cost functional*.

We note, without proof, that a closed quantum system is controllable if the matrix Lie algebra generated by the matrices $H_0, \ldots, H_m$ is SU(N)

- Approach B: find a control that brings the system as close as possible to the target, while minimizing the cost. This approach is used when the controllability step is difficult to verify. Here, the initial point is fixed and the final point is free, but the cost contains terms [denoted $d(\cdot, \cdot)$ in the next formula] that depends on the distance between the final state of the dynamics and the target:

$$\int_0^T f^0[q(t), u(t)]dt + d[\mathcal{T}, q(T)] \to \min \tag{1.6}$$

with T fixed or free.

1.3 Steps to solve an Optimal Control Problem

The steps to determine a solution to minimization problems Eq. 1.5 and Eq. 1.6 are similar to finding the minimum of a smooth function $f^0 : \mathbb{R} \to \mathbb{R}$.

1. **Find conditions that guarantee the existence of solutions.** This is crucial, if skipped, first-order conditions may provide a wrong candidate for optimality and numerical optimization schemes may either not converge or converge towards a non-minimal solution.

2. **Apply first-order necessary conditions.** This gives candidates for minima, i.e., identifies local minima, local maxima and saddles. For optimal control problems, first-order necessary conditions should be given in an infinite-dimensional space (a space of curves) and they are expressed by the PMP.

3. **Apply second-order conditions.** The step is used to further narrow down the candidates for optimality. Higher order PMP can provide these, however if difficult it can be more convenient to go directly to the next step.

4. **Selection of the best solution among all candidates.** One selects the best out of the set of candidates for optimality identified in step 1 and (perhaps) further reduced in step 2. This can be done by hand if a finite number of candidates are found. For optimal control problems, often one has infinitely many candidates making this step very difficult.

1.4 First-order Conditions

First-order conditions in optimal control are derived from the requirement that for a small control variation, there is no cost variation at first order.

1.4.1 Statement of the PMP

The basic idea is to define a new object [the pre-Hamiltonian] that allows us to formulate the Lagrange multiplier conditions simply and directly. The theorem is stated in a more general form that unifies and slightly generalizes the optimal control problems of Approaches A and B.

Particularly, we add to the cost $\int_0^T f^0[q(t), u(t)]dt$ a general terminal cost $\phi[q(T)]$. In Approach A, we have $\phi = 0$, while in Approach B, ϕ represents the distance from $q(T)$ to the target $\mathcal{T}$. We allow the target $\mathcal{T}$ to coincide with M, corresponding to leaving the final point $q(T)$ free in Approach B.

Theorem. *Consider the optimal control problem*

$$\begin{gathered} \dot{q}(t) = f[q(t), u(t)], \\ q(0) = q_{\text{in}}, \quad q(T) \in \mathcal{T}, \\ \int_0^T f^0[q(t), u(t)]dt + \phi[q(T)] \to \min, \end{gathered}$$

where

- *M is a smooth manifold of dimension n, $U \subset \mathbb{R}^m$,*
- *$\mathcal{T}$ is a (non-empty) smooth submanifold of M; it can be reduced to a point (fixed terminal point) or coincide with M (free terminal point),*
- *f, f^0 are smooth,*
- *$u \in \mathcal{U}$,*
- *$q : [0, T] \to M$ is a continuous curve.*

Define the function (called the pre-Hamiltonian)

$$\mathcal{H}(q, p, u, p^0) = \langle p, f(q, u) \rangle + p^0 f^0(q, u) \tag{1.7}$$

with

$$(q, p, u, p^0) \in T^*M \times U \times \mathbb{R}$$

If the pair $(q, u) : [0, T] \to M \times U$ *is optimal then there exists a never vanishing continuous pair* $(p, p^0) : [0, T] \ni t \mapsto [p(t), p^0] \in T^*_{q(t)}M \times \mathbb{R}$, *where* $p^0 \leq 0$ *is a constant, such that, for almost every* $t \in [0, T]$, *we have*

1. *q satisfies the Hamiltonian equation* $\dot{q}(t) = \frac{\partial \mathcal{H}}{\partial p}[q(t), p(t), u(t), p^0]$;
2. *p satisfies the Hamiltonian equation* $\dot{p}(t) = -\frac{\partial \mathcal{H}}{\partial q}[q(t), p(t), u(t), p^0]$;
3. *the quantity* $\mathcal{H}_M[q(t), p(t), p^0] := \max_{v \in U} \mathcal{H}[q(t), p(t), v, p^0]$ *is well defined and*
$$\mathcal{H}[q(t), p(t), u(t), p^0] = \mathcal{H}_M[q(t), p(t), p^0],$$
which corresponds to the maximization condition.

Moreover,

4. *there exists a constant* $c \geq 0$ *such that* $\mathcal{H}_M[q(t), p(t), p^0] = c$ *on* $[0, T]$, *with* $c = 0$ *if the final time is free (value of the Hamiltonian);*
5. *for every* $v \in T_{q(T)}\mathcal{T}$, *we have* $\langle p(T), v\rangle = p^0\langle d\phi[q(T)], v\rangle$ *(transversality condition), where* $d\phi$ *is the differential of the function* ϕ.

A few comments are necessary here.

- The covector p is called the *adjoint state* in the control theory literature, while p^0 is the *abnormal multiplier*. The quantities $p(\cdot)$ and p^0 play the roles of Lagrange multipliers for the constrained optimization problem.
- A trajectory $q(\cdot)$ for which there exist $p(\cdot), u(\cdot)$, and p^0 such that $[q(\cdot), p(\cdot), u(\cdot), p^0]$ satisfies all the conditions given by the PMP is called an *extremal trajectory* and the 4-uple $[q(\cdot), p(\cdot), u(\cdot), p^0]$ an *extremal* or, equivalently, an *extremal lift of* $q(\cdot)$.

  Such an extremal is called *normal* if $p^0 \neq 0$ and *abnormal* if $p^0 = 0$. It is possible that an extremal trajectory $q(\cdot)$ admits both a normal extremal lift $[q(\cdot), p_1(\cdot), u(\cdot), p^0]$ and an abnormal one $[q(\cdot), p_2(\cdot), u(\cdot), p^0]$. In this case, we say that the extremal trajectory $q(\cdot)$ is a *nonstrict abnormal trajectory*.

  Note that (as in the finite-dimensional case) abnormal trajectories are candidates for optimality regardless of the cost. In the finite-dimensional case, they correspond to singularities of the constraint function, while here they correspond to singularities of the functional that maps the control $v(\cdot)$ to the final point at time T of the solution of

$$\dot{q}(t) = f[q(t), v(t)], q(0) = q_{\text{in}}.$$

- The PMP is only a necessary condition for optimality. It may very well happen that an extremal trajectory is not optimal. The PMP can therefore provide several candidates for optimality, only some of which are optimal (or even none of them if the step of existence has not been verified.
- Since the equation for $p(\cdot)$ in the Theorem(2.) is linear, if $[q(\cdot), p(\cdot), u(\cdot), p^0]$ is an extremal then, for every $\alpha > 0$, $[q(\cdot), \alpha p(\cdot), u(\cdot), \alpha p^0]$ is an extremal as well.
- When there is no final cost ($\phi = 0$), the transversality condition (v) of the Theorem simplifies to

$$\langle p(T), T_{q(T)}\mathcal{T}\rangle = 0. \tag{1.8}$$

  When the final point is fixed ($\mathcal{T} = \{q_{\text{fi}}\}$), $T_{q(T)}\mathcal{T}$ is a zero-dimensional manifold, and hence, condition Eq. 1.8 is empty. When the final point is free ($\mathcal{T} = M$), the transversality condition simplifies to $p(T) = p^0 d\phi[q(T)]$. In local coordinates, we recover that $p(T)$ is proportional to the gradient of ϕ evaluated at the point $q(T)$. Note that, since $[p(T), p^0] \neq 0$, in this case one necessarily has $p^0 \neq 0$.

1.4.2 Use of the PMP

Applying the PMP is not very straightforward due to the multitude of conditions that need to be satisfied. It is made further nontrivial by their coupling to each other. Here, we describe how one can apply PMP in practice.

The following points should be followed first for normal extremals ($p^0 < 0$) and then for abnormal extremals ($p^0 = 0$). For the former, p^0 can be normalized to $-1/2$ as it is defined up to a multiplicative positive factor.

Step 1. Use the maximization condition (3.) of the Theorem to express, when possible, the control as a function of the state and of the covector, i.e., $u = w(q, p)$. If we have m controls then the first-order maximality conditions give m equations for m unknowns. When such an expression is permitted, we say that the control is *regular*; else, it is said to be *singular*. It is possible to have regions where the control is regular and regions where it is singular.

Step 2. Insert the control found in the previous step into the Hamiltonian equations 1. and 2. of the Theorem:

$$\begin{aligned} \dot{q}(t) &= \tfrac{\partial \mathcal{H}}{\partial p}\{q(t), p(t), w[q(t), p(t)], p^0\}, \\ \dot{p}(t) &= -\tfrac{\partial \mathcal{H}}{\partial q}\{q(t), p(t), w[q(t), p(t)], p^0\}. \end{aligned} \tag{1.9}$$

If the previous step provides a smooth $w(\cdot, \cdot)$, this is a well-defined set of $2n$ equations for $2n$ unknowns. However, the boundary conditions are given in a nonstandard form since we know only $q(0)$ not $p(0)$. Instead, we have

partial information on $q(T)$ and $p(T)$ depending on the dimension of $\mathcal{T}$. The next step discusses how these final conditions are shared between $q(T)$ and $p(T)$. Now, solve Eq. 1.9 for *fixed* $q(0) = q_{\text{in}}$ and *any* $p(0) = p_{\text{in}} \in T^*_{q_{\text{in}}}M$. Let us denote the solution as

$$q(t; p_{\text{in}}, p^0), \quad p(t; p_{\text{in}}, p^0)).$$

It is important to realize however, that when $w(\cdot, \cdot)$ is not regular enough, solutions to the Cauchy problem Eq. 1.9 with $q(0) = q_{\text{in}}$ and $p(0) = p_{\text{in}}$ may fail to exist or be unique.

Step 3. Find p_{in} such that

$$q(T; p_{\text{in}}, p^0) \in \mathcal{T}. \tag{1.10}$$

If $\mathcal{T}$ is reduced to a point and T is fixed, we get n equations for n unknowns (the components of p_{in}). If T is free then an additional equation is needed. This condition is given by 4. in the PMP. If $\mathcal{T}$ is a k-dimensional submanifold of M ($k \leq n$) then Eq. 1.10 provides only $n - k$ equations and the remaining ones correspond to the transversality condition 5. of the PMP.

Step 4. If Eq. 1.10 [together with the transversality condition and condition 4. of the PMP if T is free] has a unique solution p_{in} and if we have *a priori* verified the existence of an optimal solution, then the optimal control problem is solved.

Unfortunately, in general, there is no reason for Eq. 1.10 to have a unique solution. The PMP is only a necessary condition for optimality. If several solutions are found, one must choose the best by directly comparing the value of their cost. This, in general, can be a nontrivial step, complicated by the difficulty of explicitly solving Eq. 1.10. Hence, several techniques have been developed to select the extremals.

1.4.3 An expository example

As a general example in quantum control, consider a dynamical system governed by Eq. 1.2 where the goal is to minimize at the fixed final time T, the cost $-|\langle\psi_{\text{fi}}|\psi(T)\rangle|^2 + \frac{1}{2}\int_0^T \sum_{j=1}^m u_j^2(t)dt$, where ψ_{fi} is a target state towards which we wish to drive our system (up to a global phase).

A direct application of the PMP shows that the pre-Hamiltonian $\mathcal{H}$ can be expressed as

$$\mathcal{H}(\psi, \chi, u_j, p^0) = \text{Re}(\langle\chi|\dot{\psi}\rangle) + \frac{p^0}{2}\sum_j u_j^2,$$

where the adjoint state (χ) is an abstract wavefunction that can be chosen to belong to the unit sphere in $\mathbb{C}^N$, $\langle\chi|\chi\rangle = 1$. As ψ and χ are complex-valued

functions, the pre-Hamiltonian is defined through the real part of the scalar product between χ and $\dot{\psi}$. If we introduce the real and imaginary parts of the wavefunctions, we can use Eq. 1.2 to get

$$\mathcal{H}(\psi, \chi, u_j, p^0) = \mathrm{Im}\left(\langle \chi | H_0 + \sum_j u_j H_j | \psi \rangle\right) + \frac{p^0}{2} \sum_j u_j^2, \tag{1.11}$$

which leads to

$$i\dot{\chi}(t) = \left(H_0 + \sum_{j=1}^{m} u_j(t) H_j\right) \chi(t),$$

i.e., χ also satisfies the Schrödinger equation, note however, that this condition is only true in the bilinear case. The final condition $\chi(T)$ is given by the transversality condition 5. of the PMP:

$$\chi(T) = p^0 \langle \psi_{\mathrm{fi}} | \psi(T) \rangle \psi_{\mathrm{fi}}. \tag{1.12}$$

The maxima condition of the PMP leads us to the constraints

$$\frac{\partial \mathcal{H}}{\partial u_j}(\psi, \chi, u_j, p^0) = 0$$

for $j = 1, \ldots, m$. A direct computation from Eq. 1.11 gives

$$\mathrm{Im}(\langle \chi | H_j | \psi \rangle) + p^0 u_j = 0.$$

For the normal extremal with $p^0 = -1$, we finally get

$$u_j = \mathrm{Im}(\langle \chi | H_j | \psi). \tag{1.13}$$

We have shown with Eq. 1.13 that the maximization condition allows us to express the m controls u_j as functions of ψ and χ in the normal case. This situation corresponds to Step 1 and above where the control is regular. For abnormal extremals for which $p^0 = 0$, we get

$$\mathrm{Im}(\langle \chi | H_j | \psi \rangle = 0,) \tag{1.14}$$

and the control is singular because this relation does not directly give the expression for u_j.

Applying Step 2, in the regular situation we can get the following coupled equations for ψ and χ:

$$\begin{aligned} i\dot{\psi} &= \left[H_0 + \textstyle\sum_j \mathrm{Im}(\langle \chi | H_j | \psi \rangle) H_j\right] \psi, \\ i\dot{\chi} &= \left[H_0 + \textstyle\sum_j \mathrm{Im}(\langle \chi | H_j | \psi \rangle) H_j\right] \chi. \end{aligned} \tag{1.15}$$

with the boundary conditions $\psi(0) = \psi_{\mathrm{in}}$ and Eq. 1.12. In Step 3, we then solve Eq. 1.15 to find the initial condition $\chi(0)$ such that the final state $\chi(T)$

satisfies Eq. 1.12 at time T.

The numerical procedures used to select the initial condition $\chi(0)$, called *shooting methods* in control theory, are based on suitable adaptations of the Newton algorithm. Some thoughts on this matter are shared near the end of this report. Step 4 then consists of finally comparing the cost of the different solutions found in Step 3.

In the abnormal case, we use the fact that Eq. 1.14 is satisfied in a nonzero time interval, so the time derivatives of $\mathrm{Im}(\langle\chi|H_j|\psi\rangle)$ are also zero. The first time derivative leads to the m relations

$$\sum_{j=1}^{m} u_j \,\mathrm{Re}(\langle\chi|[H_k, H_j]|\psi = \mathrm{Re}(\langle\chi|[H_0, H_k]|\psi)$$

with $k = 1, \ldots, m$. This linear system can be expressed in a more compact form as

$$Ru = s,$$

where R is an $m \times m$ matrix with elements $R_{kj} = \mathrm{Re}(\langle\chi|[H_k, H_j]|\psi\rangle)$ and s a vector of coordinates $s_k = \mathrm{Re}(\langle\chi|[H_0, H_k]|\psi\rangle)$.

It is evident that the control u is given as a function of ψ and χ as $u = R^{-1}s$. For a singular system, the second derivative must be used. This occurs, e.g., for $m = 1$, when a further constraint has to be fulfilled, namely, $\mathrm{Re}(\langle\chi|[H_0, H_1]|\psi) = 0$. From the derivation of u, we can apply Steps 2 and 3 to the abnormal extremals.

1.5 Gradient-based Optimization Algorithm

This section introduces a first-order gradient-based optimization algorithm based on the PMP. First, the necessary conditions of the PMP for the case of a fixed control time without constraints on final state and control. In control theory, such a construction is known as the weak PMP. We only consider the case of regular control. From these conditions we can derive iterative algorithms, this idea is applied to quantum control to design a gradient-based optimization algorithm, GRAPE, a pioneering mainstay of quantum optimal control.

1.5.1 The weak PMP

Consider a control system with dynamics governed by Eq. 1.1 when the final state is free and the control is unconstrained. Our objective is to solve a control problem using Approach B for a fixed control time T. Recall the cost functional to be minimized can be written as

$$J[u(\cdot)] = \int_0^T f^0[q(t), u(t)]dt + d[\mathcal{T}, q(T)].$$

Taking the evolution equation Eq. 1.1 as a dynamical constraint (in infinite dimension), to formally apply the Lagrange multiplier rule for normal extremals, we introduce the functional

$$\Lambda[p(\cdot), u(\cdot)] = \begin{array}{l} d[\mathcal{T}, q(T)] + \int_0^T f^0[q(t), u(t)]dt \\ + \int_0^T \langle p(t), \dot{q}(t) - f[q(t), u(t)]\rangle dt. \end{array} \tag{1.16}$$

It is important to note here that the Lagrange multiplier $p(\cdot)$ is a function on $[0, T]$. We can then integrate Eq. 1.16 by parts to get

$$\Lambda[p(\cdot), u(\cdot)] = \begin{array}{l} d[\mathcal{T}, q(T)] + \langle p(T), q(T)\rangle - \langle p(0), q(0)\rangle \\ - \int_0^T \{H[q(t), p(t), u(t)] + \langle \dot{p}(t), q(t)\rangle\} dt \end{array}$$

with

$$H(q, p, u) = \langle p, f(q, u)\rangle - f^0(q, u). \tag{1.17}$$

Here, the scalar function H has the same expression as the pre-Hamiltonian $\mathcal{H}$ introduced in the statement of the PMP with $p^0 = -1$. As we do not have any constraint on the control law, i.e., $u(t) \in \mathbb{R}^m$ for any time t, we consider the variation $\delta\Lambda$ in Λ at first order due to the variation δu of u. This change of control induces a variation of trajectory $\delta q(t)$ with $\delta q(0) = 0$, as the initial point is fixed. Note however that the adjoint state p is not modified. Thus, we arrive at

$$\delta\Lambda = \begin{array}{l} \left\langle \frac{\partial d(\mathcal{T}, q)}{\partial q} \mid_{q=q(T)} + p(T), \delta q(T) \right\rangle \\ - \int_0^T \left[\left\langle \frac{\partial H}{\partial q} + \dot{p}, \delta q \right\rangle + \frac{\partial H}{\partial u} \delta u \right] dt. \end{array} \tag{1.18}$$

A necessary condition for Λ to be an extremum is $\delta\Lambda = 0$ for any variation δu. For a solution, we take an adjoint state p satisfying

$$\dot{p} = -\frac{\partial H}{\partial q}, \tag{1.19}$$

the final boundary condition

$$p(T) = -\frac{\partial d(\mathcal{T}, q}{\partial q} \mid_{q=q(T)}, \tag{1.20}$$

and requiring that

$$\frac{\partial H}{\partial u} = 0 \text{ on } [0, T].$$

As expected, these are a weaker variant of the equations of the PMP introduced earlier where the maximization of the pre-Hamiltonian is replaced by an extremum condition given by the partial derivative with respect to u. Note that this approach works if the set U is open.

1.5.2 Gradient-based optimization algorithm

The set of nonlinear coupled differential equations can be numerically solved by an iterative algorithm. The basic idea in such approaches can be formulated as follows. Assume a control $u(\cdot)$ sufficiently close to the optimal solution is known. If $p(\cdot)$ satisfies Eqs. 1.19 and 1.20 then from Eq. 1.18 we get

$$\delta\Lambda = -\int_0^T \frac{\partial H}{\partial u}\delta u dt.$$

This suggests that better control can be achieved with the choice $\delta u = \epsilon\partial H/\partial u$, where ϵ is a small positive parameter. The following steps describe the iterative algorithm.

1. Choose a guess control $u(\cdot)$.
2. Propagate forward the state of the system q from $\dot{q} = f(q,u)$, with the initial condition $q(0) = q_0$.
3. Propagate backward the adjoint state of the system from $\dot{p} = -\partial H/\partial q$, with the final condition $p(T) = -\partial d(\mathcal{T},q)/\partial q|_{q=q(T)}$.
4. Compute the correction δu to the control law, $\delta u(t) = \epsilon\partial H/\partial u$, where $\epsilon > 0$ is a small parameter.
5. Define the new control $u \mapsto u + \delta u$.
6. Go to Step 2. and repeat until a given accuracy is reached.

This is an example of a first-order gradient-based optimization algorithm. By construction, it converges towards an extremal control of J that is not, necessarily, a global minimum solution of the control problem, only a local one. The choice of the guess control and the parameter ϵ are crucial to arrive at a good local solution and remain in the first-order approximation.

This approach can be directly applied to quantum systems taking advantage of the bilinearity of quantum dynamics to simplify various terms in the algorithm. Consider a quantum system whose dynamics are governed by the Schrödinger equation

$$i\dot{\psi}(t) = [H_0 + u(t)H_1]\psi(t).$$

The goal of the control process is to bring the system from ψ_{in} towards ψ_{fi} in a fixed time T. The control problem attempts to minimize the cost

$$J = \frac{1}{2}\int_0^T u(t)^2 dt - |\langle\psi_{\text{fi}}|\psi(T)\rangle|vert^2.$$

In the normal case, the pre-Hamiltonian H can be expressed as

$$H = \text{Re}[\langle\chi|\dot{\psi}\rangle] - \frac{u^2}{2} = \text{Im}[\langle\chi|H_0 + uH_1|\psi\rangle] - \frac{u^2}{2},$$

where the wave function χ is the adjoint state of the system. We have thus deduced that the gradient on which the iterative algorithm is based on is given by

$$\frac{\partial H}{\partial u} = \mathrm{Im}[\langle \chi | H_1 | \psi \rangle] - u(t). \tag{1.21}$$

Eq. 1.21 is the standard control correction used in the GRAPE algorithm in quantum control. A newer optimal control protocol with a simpler mechanism to calculate the gradient update is the GOAT algorithm (gradient optimization of analytic controls) (Machnes et al., 2018).

2 Discrete Time Pontryagin Maximum Principle

The Pontryagin maximum principle (PMP) provides first-order necessary conditions for a broad class of optimal control problems. These necessary conditions typically lead to two-point boundary value problems that characterize optimal control, and these problems may be solved to arrive at the optimal control functions. This approach is widely applied to solve optimal control problems for controlled dynamical systems that arise in various fields of engineering including robotics, aerospace and quantum mechanics.

Here we follow (Paruchuri et al., 2020; Paruchuri and Chatterjee, 2019; Phogat, Chatterjee, and Banavar, 2018) to present a geometric discrete-time Pontryagin maximum principle (PMP) on matrix Lie groups, that incorporates frequency constraints on the controls in addition to pointwise constraints on the states and control actions directly at the stage of the problem formulation.

2.1 Motivation

2.1.1 Need for a discrete-time PMP

Constrained optimal control problems for nonlinear continuous-time systems can, in general, be solved only numerically, and two technical issues inevitably arise.

First, the accuracy guaranteed by a numerical technique largely depends on the discretization of the continuous-time system underlying the problem. For control systems evolving on complicated state spaces such as manifolds, preserving the manifold structure of the state space under discretization is a nontrivial matter.

Second, classical versions of the PMP apply only to optimal control problems in which the dynamics evolve on Euclidean spaces and do not carry over directly to systems evolving on more complicated manifolds. Thus, numerical solutions to optimal control problems, via digital computational means, need a discrete-time PMP.

2.1.2 State-Action-Frequency Constraints

Most engineering systems are required to operate in a certain pre-defined region of the state and control spaces. For instance, since mechanical systems are inertial, mechanical actuators have natural limitations in terms of, e.g., the torque magnitudes and the operating frequencies. In the control literature, these are known as control magnitude and frequency constraints, respectively.

Control magnitudes must be limited, for instance, to prevent rapid movements of robotic arms for safety considerations. Frequency constraints arise from a more subtle consideration. Consider, for instance, attitude orientation manoeuvres of satellites fitted with flexible structures such as solar panels may excite the natural frequencies of the flexible structures, leading to vibrations and structural damage unless the natural frequencies are avoided. It is, therefore, desirable to eliminate certain frequencies from the spectra of the control functions of controlled systems at the control synthesis stage.

In the context of quantum control, quantum systems often have particular resonant modes that introduce significant errors if excited. For engineered superconducting qubits operated using microwave control signals, these may include other spurious two-level systems in the substrate, higher energy level transitions out of the two-state computational subspace or even other qubits that may be exposed to this signal that we do not wish to operate on. Further, the configuration variables of a quantum system evolve on matrix Lie groups, making this effort natively applicable.

We present a technique to find *tractable* solutions to optimal control problems that simultaneously incorporate an entire class of hard constraints on the states, control actions and frequency constraints on the control trajectories, right at the synthesis stage. The conditions for optimality then give rise to constrained two-point boundary value problems that can be solved via multiple shooting techniques. These are discussed in more detail in the following chapter, but they can be implemented on a parallel architecture for fast computation.

2.2 Problem setup

Let us fix a positive integer N that plays the role of a time horizon, and for $\mathcal{N} \in \mathbb{N}^*$, set $[\mathcal{N}] := \{0, \dots, \mathcal{N}-1\}$ and $[\mathcal{N}]^* := [\mathcal{N}] \setminus \{0\}$. Let G be a matrix Lie group with $\mathfrak{g}$ its Lie algebra; the map $\exp : \mathfrak{g} \to G$ denotes the corresponding exponential map. Recall that for each $X \in \mathfrak{g}$, there exists a map $\exp^X(\cdot) : \mathbb{R} \to G$ such that $\exp^X(0) = e \in G$, $\partial_t|_{t=0} \exp^X(t) = X$, and $\exp^X(t+s) = \exp^X(t)\exp^X(s)$, where e is the group identity. For $y \in \mathbb{C}^N$ we let $\mathrm{supp}(y) := \{i \in [N]^* | y_i \neq 0\}$.

Consider a controlled discrete-time system evolving partly on a fixed matrix Lie group G and partly on $\mathbb{R}^d$, given by

$$\begin{cases} q_{t+1} &= q_t s_t(q_t, x_t) \\ x_{t+1} &= f_t(q_t, x_t, u_t) \end{cases} \text{ for } t \in [N]^*, \tag{2.1}$$

where $(q_t, x_t) \in G \times \mathbb{R}^d$ is the vector of states and $u_t \in \mathbb{R}^m$ the vector of control actions of the system at a discrete-time instant t. The maps $s_t : G \times \mathbb{R}^d \to G$ (describing the dynamics of the states q_t on the matrix Lie group G) and $f_t : G \times \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R}^d$ (describing the dynamics of state x_t in $\mathbb{R}^d$) are smooth. Assume further that there exists an open set $\mathcal{O} \subset \mathfrak{g}$ such that the following conditions hold:

1. the exponential map $\exp : \mathcal{O} \to \exp(\mathcal{O})$ is a diffeomorphism, and
2. the image of s_t is a subset of $\exp(\mathcal{O})$ for all t.

An open set $\mathcal{O}$ satisfying condition 1. always exists by definition of the exponential map but condition 2. is an *assumption* that stipulates that the time-discretization step is sufficiently small.

2.2.1 Frequency constraints

Let us briefly discuss discrete-time control frequency constraints. Let $\mathbb{R}^N \ni u^{(k)} := (u_t^{(k)})_{t=0}^{N-1}$ be the trajectory of the k^{th} component of the control. Throughout the rest of this report, the subscript on u denotes the stage and the superscript denotes the component of the control. The hat on top of a variable denotes its frequency representation. The discrete Fourier transform (DFT) of $u^{(k)}$ is defined by

$$\mathbb{C}^N \ni \widehat{u^{(k)}} := \boldsymbol{F} u^{(k)} \quad \text{for } k = 1, \dots, m,$$

$$\text{where } \boldsymbol{F} := \frac{1}{\sqrt{N}} \left(\begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega & \cdots & \omega^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \cdots & \omega^{(N-1)(N-1)} \end{bmatrix} \right) \in \mathbb{C}^{N \times N}$$

for $\omega := \mathrm{e}^{\frac{-i2\pi}{N}}$. Let u denote the stacked vector $\left((u^{(1)})^\top \dots (u^{(m)})^\top \right)^\top$, and define the DFT of a control trajectory by the vector

$$\mathbb{C}^{mN} \ni \hat{u} := \left(\begin{bmatrix} \widehat{u^{(1)}} \\ \vdots \\ \widehat{u^{(m)}} \end{bmatrix} \right) = \left(\begin{bmatrix} \boldsymbol{F} u^{(1)} \\ \vdots \\ \boldsymbol{F} u^{(m)} \end{bmatrix} \right) = \mathcal{F} \left(\begin{bmatrix} u^{(1)} \\ \vdots \\ u^{(m)} \end{bmatrix} \right),$$

where $\mathcal{F}$ is a block diagonal matrix with the standard DFT matrix $\boldsymbol{F}$ being each block. Note here that $(\widehat{u^{(k)}})_j \in \mathbb{C}$ represents the $(2\pi(j-1)/N)^{\text{th}}$ frequency component of the trajectory $u^{(k)}$. Hence, if elimination of the $(2\pi(j-1)/N)^{\text{th}}$ frequency component of $u^{(k)}$ is desired, it can be ensured by introducing the constraint

$$0 = (\widehat{u^{(k)}})_j = \boldsymbol{F}_j u^{(k)},$$

where $\boldsymbol{F}_j$ is the j^{th} row of the DFT matrix defined above. Hence, in general, control frequency constraints can be enforced by a collection of affine equality conditions in the control action variables, and this is represented abstractly by one equality constraint

$$\sum_{t=0}^{N-1} \widetilde{F}_t u_t = 0 \quad \text{where } \widetilde{F}_t \text{ are suitable matrices.} \tag{2.2}$$

It is imperative to point out here that how frequency constraints have been assimilated into the problem formulation enables the designer to cancel particular frequencies in the control inputs, a feature distinctly absent in other control synthesis schemes. Particularly for quantum control applications, specific resonant excitations can be avoided that trigger spurious unwanted systems in the substrate or higher levels in a truncated harmonic oscillator.

2.2.2 Constrained optimal control problem

Collecting the definitions above, our constrained optimal control problem in discrete-time is:

$$\begin{aligned} &\underset{(u_t)_{t=0}^{N-1}}{\text{minimize}} \quad \textstyle\sum_{t=0}^{N-1} c_t(q_t, x_t, u_t) + c_N(q_N, x_N) \\ &\text{subject to} \quad \begin{cases} \text{dynamics (2.1)}, \\ u_t \in \mathbb{U}_t \quad \text{for each } t \in [N], \\ \varphi_t(q_t, x_t) \leqslant 0 \text{ for each } t \in [N+1]^* \\ (q_0, x_0) = (\bar{q}, \bar{x}), \\ F(u_0, \ldots, u_{N-1}) = 0, \end{cases} \end{aligned} \tag{2.3}$$

with the following data:

1. $(\bar{q}, \bar{x}) \in G \times \mathbb{R}^d$ and $N \in \mathbb{N}$ are fixed;
2. the maps $c_t : G \times \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R}$ (for each $t \in [N]$ defining the cost-per-stage) and $c_N : G \times \mathbb{R}^d \to \mathbb{R}$ (accounting for the final stage cost) are smooth;
3. the maps $\varphi_t : G \times \mathbb{R}^d \to \mathbb{R}^{n_t}$ for $t \in [N+1]^*$ denote constraints on the states and are smooth;
4. the set of admissible control actions $\mathbb{U}_t \subset \mathbb{R}^m$ is convex and compact for each $t \in [N]$;
5. the linear map $\mathbb{R}^{mN} \ni (u_0, \ldots, u_{N-1}) \mapsto F(u_0, \ldots, u_{N-1}) := \sum_{t=0}^{N-1} \tilde{F}_t u_t \in \mathbb{R}^\ell$ represents constraints on the frequency components of the control profile $(u_t)_{t=0}^{N-1}$.

Here, the map F as defined in 5. provides the real and imaginary components of the required frequency components of the control profile. For the special case of eliminating certain frequency components, we can simply set the constraint $F(u_0, \dots, u_{N-1}) = 0$ in 2.3. However, this approach can be extended to a larger class of constraints on the frequency components.

We shall now borrow a few definitions from the theory of Lie groups to state the main result. Let $G \ni q \mapsto h(q) \in \mathbb{R}$ be a function defined on a manifold G. The *tangent lift* of the function h at a point $q_0 \in G$ is the map

$$T_{q_0}G \ni v \mapsto \mathcal{D}_q h(q_0)v := \partial_t|_{t=0} h(\gamma(t)) \in \mathbb{R},$$

where $\gamma(t)$ is a path in the manifold G with $\gamma(0) = q_0$ and $\partial_t|_{t=0}\gamma(t) = v$.

Let $\Phi : G \times G \to G$ be a *left action* and let $\Phi_g : G \to G$ denote $\Phi(g, \cdot)$. The *tangent lift* of Φ, $T\Phi : G \times TG$ is the action

$$(g, (h, v)) \mapsto T\Phi_g(h, v) = (\Phi_g(h), T_h\Phi_g(v)), \quad (h, v) \in T_hG.$$

The *cotangent lift* of Φ, $T^*\Phi : G \times T^*G \to T^*G$, is the action

$$(g, (h, a)) \mapsto T^*\Phi_{g^{-1}}(h, a) = (\Phi_g(h), T^*_{\Phi_g(h)}\Phi_{g^{-1}}(a), a \in T^*_hG.$$

The *adjoint action* of G on $\mathfrak{g}$ is defined as

$$G \times \mathfrak{g} \ni (g, \beta) \mapsto \mathrm{Ad}_g\, \beta := \partial_s|_{s=0} g\, \mathrm{e}^{s\beta}\, g^{-1} \in \mathfrak{g},$$

and finally, the *co-adjoint action* of G on $\mathfrak{g}^*$ is the inverse dual of the adjoint action, given by

$$G \times \mathfrak{g}^* \ni (g, a) \mapsto \mathrm{Ad}^*_{g^{-1}}\, a \in \mathfrak{g}^*,$$

where $\left\langle \mathrm{Ad}^*_{g^{-1}}\, a, \beta \right\rangle = \left\langle a, \mathrm{Ad}_{g^{-1}}\, \beta \right\rangle$.

2.3 The main theorem

Theorem. *Let $(u^o_t)_{t=0}^{N-1}$ be an optimal control trajectory for 2.3 and $(q^o_t, x^o_t)_{t=0}^{N}$ be the corresponding state trajectory. Define the (pre-)Hamiltonian*

$$\begin{aligned}\mathfrak{g} \times \mathbb{R}^d \times [N]^* \times G \times \mathbb{R}^d \times \mathbb{R}^m \ni (\varrho, \zeta, \tau, v, \xi, \mu) \mapsto H^{v,\vartheta}(\varrho, \zeta, \tau, v, \xi, \mu) \\ := vc_\tau(v, \xi, \mu) + \left\langle \varrho, \exp^{-1}\left(s_\tau(v, \xi)\right)\right\rangle_{\mathfrak{g}} + \langle \zeta, f_\tau(v, \xi, \mu)\rangle + \left\langle \vartheta, \widetilde{F}_\tau \mu \right\rangle \in \mathbb{R}.\end{aligned} \tag{2.4}$$

Then there exist

- *adjoint trajectories $(\eta^f_t)_{t=0}^{N-1} \subset \mathbb{R}^d$, $(\eta^g_t)_{t=0}^{N-1} \subset \mathfrak{g}$,*
- *covectors $\eta^X_t \in \mathbb{R}^{n_t}$ for $t \in [N+1]^*$, and*
- *a pair $(\eta^c, \hat{\eta}) \in \{-1, 0\} \times \mathbb{R}^\ell$*

such that the following conditions hold with $\gamma_t^o := (\eta_t^g, \eta_t^f, t, q_t^o, x_t^o, u_t^o)$ *and* $\beta_t^g := (\mathcal{D}\exp^{-1}((q_t^o)^{-1}q_{t+1}^o) \circ T_e\Phi_{(q_t^o)^{-1}q_{t+1}^o})^*(\eta_t^g)$*:*

1. *the non-triviality condition: the adjoint variables* $(\eta_t^f)_{t=0}^{N-1}$, $(\eta_t^g)_{t=0}^{N-1}$, *and the pair* $(\eta_c, \hat{\eta})$ *do not simultaneously vanish;*

2. *the state and adjoint dynamics:*

$$\begin{array}{ll} \textit{state} & \begin{cases} q_{t+1}^o &= q_t^o \exp\left(\mathcal{D}_\varrho H^{\eta^c,\hat{\eta}}(\gamma_t^o)\right), \\ x_{t+1}^o &= \mathcal{D}_\xi H^{\eta^c,\hat{\eta}}(\gamma_t^o), \end{cases} \\ \textit{adjoint} & \begin{cases} \beta_{t-1}^g &= T_e^*\Phi_{q_t^o}\left(\mathcal{D}_v H^{\eta^c,\hat{\eta}}(\gamma_t^o) + \eta_t^X \mathcal{D}_v\varphi_t(q_t^o, x_t^o)\right) \\ &\quad + \mathrm{Ad}^*_{\exp\left(\left(\mathcal{D}_\varrho H^{\eta^c,\hat{\eta}}(\gamma_t^o)\right)\right)}\beta_t^g, \\ \eta_{t-1}^f &= \mathcal{D}_\xi H^{\eta^c,\hat{\eta}}(\gamma_t^o) + \eta_t^X \mathcal{D}_\xi\varphi_t(q_t^o, x_t^o); \end{cases} \end{array}$$

3. *the transversality conditions:*

$$\begin{aligned} \beta_{N-1}^g &= T_e^*\Phi_{q_N^o}\left(\eta^c\mathcal{D}_v c_N(q_N^o, x_N^o) + \eta_N^X\mathcal{D}_v\varphi_N(q_N^o, x_N^o)\right), \\ \eta_{N-1}^f &= \eta^c\mathcal{D}_\xi c_N(q_N^o, x_N^o) + \eta_N^X\mathcal{D}_\xi\varphi_N(q_N^o, x_N^o); \end{aligned}$$

4. *the (pre-)Hamiltonian non-positive gradient condition:*

$$\left\langle \mathcal{D}_\mu H^{\eta^c,\hat{\eta}}(\gamma_t^o), w - u_t^o \right\rangle \leqslant 0 \quad \textit{for all } w \in \mathbb{U}_t;$$

5. *the complementary slackness conditions:*

$$\begin{aligned} &(\eta_t^X)^{(j)}\varphi_t^{(j)}(q_t^o, x_t^o) = 0 \\ &\quad \textit{for all } j \in [n_t + 1]^* \textit{ and } t \in [N+1]^* \end{aligned}$$

6. *the non-positivity condition*

$$\eta_t^X \leqslant 0 \quad \textit{for all } t \in [N+1]^*.$$

Here, the adjoint variables (a.k.a 'multipliers') corresponding to the cost, the dynamics, the state constraints, and the frequency constraints of the control trajectories appear, and they are distinguished by introducing various super-scripts of the single Greek letter η. Objects in frequency space are distinguished by a 'hat'. In particular, the two adjoint variables that are constant with time appear in the superscript of the (pre-)Hamiltonian.

3 Shooting Techniques

In spirit, the first-order necessary conditions for optimality are similar to the classical Euler's necessary conditions for optimality (that states that the gradient of a smooth function defined on an open set must vanish at an extremum point). Numerical algorithms are thereafter needed to arrive at optimal solutions starting from the necessary conditions given by the PMP. Our problem of finding a solution of the OCP characterized by the PMP can be reduced to finding a zero of a *nonlinear and implicit function*. In this chapter, we briefly review two classes of shooting techniques that can be called upon to solve this root-finding problem posed by the resulting two-point boundary value problem distilled from the PMP. One is gradient-based and one is stochastic.

3.1 Newton-Raphson

The algorithms typically employed in computing a zero of a nonlinear map Φ are based on the Newton-Raphson (NR) iterative scheme and continuation methods. Here, we follow (Hesse, 2008). Recall that the NR iterates starts with the intention of finding a zero of the first-order approximation of Φ near a zero ζ of Φ, i.e., from the affine map $z' \mapsto \Phi(z) + \Phi'(z)(z' - z)$ for z, z' sufficiently close to ζ, leading to the recursion $z_{k+1} = z_k - \Phi'(z_k)^{-1}\Phi(z_k)$ for $k = 0, 1, \ldots$.

Under standard hypotheses the sequence $(z_k)_{k\in\mathbb{N}}$ of iterates converges to ζ. The effectiveness of the NR scheme is highly dependent on

- the map Φ being sufficiently smooth,
- the availability of a good initial guess of the joint state-adjoint variables at one of the boundary points of the interval,
- the need for the derivative of Φ to be invertible everywhere sufficiently close to a zero of Φ, and
- the accuracy of the numerical computation of the derivative of Φ via finite-difference schemes.

The lack, in general, of a large enough region of convergence is a well-documented issue with the NR scheme. Further, as Φ is nonlinear and implicitly defined in our setting, this smoothness and by extension its differentiability are difficult to ascertain *a priori*, which makes it difficult to verify the hypotheses of the NR scheme. Hence, the need for an algorithm that is

"derivative-free" is acute. However, if the NR scheme *does* converge, then it converges *quadratically*, which is a highly desirable property.

3.2 Robbins-Monro

The need for a derivative-free root-finding algorithm brings us to the Robbins-Monro (RM) scheme, also known as Stochastic Approximation (SA). Stochastic approximation has been one of the main workhorses of statistical computation for many decades. It only relies on the ability to evaluate the function at given points. Here we follow an excellent, accessible introduction (Borkar, 2013). First introduced by Herbert Robbins and his student Sutton Monro in 1951. Its popularity can be attributed to the pervasiveness of 'noise' or randomness in engineering systems and the scheme's adaptability to work in noisy situations. Another reason could be its *incremental* nature that garnered several advantages including lower per iterate computation and memory requirements. SA 'adapts' to the needs of the problem.

Consider the problem of finding the root(s) of a nonlinear function $h : \mathbb{R}^d \mapsto \mathbb{R}^d$ given only noisy measurements. It can be considered as a black box that on input $x \in \mathbb{R}^d$ gives out $h(x) +$ noise. The Robbins-Monro scheme is the d-dimensional iteration

$$x_{n+1} = x_n + a(n)[h(x_n) + M_{n+1}], \tag{3.1}$$

initiated at some x_0. Here, the 'noise' $\{M_n\}$ is considered to be uncorrelated with the past which is intuitively consistent. It is important to note here that this iteration scales only *linearly* with the problem size, a much-desired advantage over alternative methods. The entire term in the square brackets is what is measured, we *do not* know $h(x_n)$ and M_{n+1} independently. The master stroke of Robbins and Monro was to choose the step-size sequence $a(n) > 0$ such that

$$\sum_n a(n) = \infty, \quad \sum_n a(n)^2 < \infty. \tag{3.2}$$

This can be understood as having a 'fat tail' and finite energy. Let us use the 'ODE' (for 'Ordinary Differential Equations') approach developed by Derevitskii and Fradkov in the USSR to analyse the power of this scheme. The iteration 3.1 can be considered a noisy discretization (or 'Euler scheme') for the ODE

$$\dot{x}(t) = h(x(t)) \tag{3.3}$$

with decreasing step-sizes $\{a(n)\}$ and noise $\{M_n\}$. Recall that the Euler scheme for numerically solving 3.3 on a computer is $x_{n+1} = x_n + ah(x_n)$ for a step-size $a > 0$. We here replace the constant a with the decreasing sequence $a(n), n \geq 0$, and $h(x_n)$ by its noisy measurement $h(x_n) + M_{n+1}$.

One can show that with probability one, x_n as $n \to \infty$ will have the same asymptotic behaviour as 3.3. 3.2 allows us to treat $\{a(n)\}$ as discrete time steps and the entire time axis is covered when we track the asymptotic behaviour of 3.3 as time tends to infinity. This also ensures that the errors due to discretization and noise are asymptotically negligible because it is ensured that $a(n)$, which is both the discretization step *and* a weight for the noise at time n, decreases to zero at a certain minimum rate. Recall that an equilibrium of 3.3 is a point x^* such that $h(x^*) = 0$ when the constant trajectory $x(t) - x^*$ is a valid solution of 3.3 i.e., if 3.3 has a unique asymptotically stable equilibrium x^*, then $x_n \to x^*$ with probability one.

SA 'generalizes' the strong law of large numbers in a sense: it 'averages out' the noise. While the case of a unique globally asymptotically stable equilibrium is very special, it is not necessarily ensured in all applications. If the noise is sufficiently 'rich', the unstable equilibria, i.e., any with some directions along which nearby trajectories move away, are avoided with probability one. This is called 'avoidance of traps'. However, all stable equilibria, not necessarily all desirable, can have strictly positive probability. The RM iteration can be implemented in a distributed fashion with different processors or agents implementing different components. With some overhead of additional complications, this can speed up implementation as the liming dynamics are unaffected and any new fluctuations are 'squeezed out' by the time scaling implicit in the decreasing step sizes. One can also deliberately use different step sizes for different components. Smaller steps ensure graceful convergence at the expense of speed, additional averaging similarly reduces fluctuations at the expense of speed. The most common application is $h(\cdot) = -\nabla F(\cdot)$, arising from trying to minimize a function $F(\cdot)$ given noisy measurements of its gradient.

3.3 A hybrid technique

Here, we follow (Kumar et al., 2022) and discuss a recent recursive algorithm that combines the SA algorithm and the NR scheme to find a zero of Φ. This hybrid algorithm combines some of the best features of the SA algorithm, namely, the exploration of space to find a zero, the ability to progress without derivative computations, etc., with the best features of the NR scheme, namely, a fast (quadratic) rate of convergence.

1. The SA algorithm is first employed to converge sufficiently close to a zero of Φ, ensured by the difference between several successive steps of the recursions being bounded above by a sufficiently small threshold preassigned by the designer. This serves an exploratory purpose to find a suitable neighbourhood of a zero of Φ to settle down and provide a warm start for the next step.

2. Switch to the NR scheme (or a suitable variant) with the final iterate of the SA algorithm being the initial condition of the NR iterations. The

idea is that since the NR scheme typically suffers from small regions of convergence, the SA takes care of the hunt for suitable initial guesses. As the NR iterates must converge quadratically, it is clear after only a few observations of its iterates whether they show signs of convergence. This means whether *scalars* $\|\Phi(z_k)\|$ and $\|z_k - z_{k-1}\|$ decrease on an average speed over several successive iterates k. Further, higher order finite difference schemes can be employed to compute the gradient matrix $\mathbb{G}$ of the function $z \mapsto \Phi(z)$ since an explicit expression of Φ is unavailable (a standard situation in shooting methods in optimal control).

3. If these iterates indeed converge, continue with the NR iteration to obtain a zero. Otherwise, simply revert to the SA algorithm in Step 1. above, continue with the iterations with a smaller threshold of error, and repeat until convergence.

4 Conclusion

4.1 A Brief Summary

In this report, we have reviewed the application of optimal control to quantum control problems using the Pontryagin Maximum Principle. The dynamics were formulated, a framework to solve the OCP and the first-order condition for optimality in the form of the PMP were discussed and applied in an expository example. The connection between PMP and GRAPE was outlined.

We then reviewed recent modifications to the PMP for application in discrete time dynamics, constraints on states, actions and frequencies of control inputs and its application on Lie groups (the natural setting for quantum mechanics). The PMP provides a two-point boundary value problem that can be reduced to a root-finding problem of a nonlinear implicit function. Shooting techniques based on stochastic and gradient-based approaches are discussed before a short presentation of a hybrid protocol to incorporate the best of both approaches.

4.2 Future Avenues

In future work, we seek to implement the frequency-constrained discrete PMP as presented in (Paruchuri et al., 2020) to quantum optimal control problems as exemplified for the standard PMP in Chapter 1. We will attempt to solve the two-point BVP using the NR, RM and hybrid approaches and draw a comparative analysis. We plan to use software tools like CasADi (Andersson et al., 2019) for a framework to describe the optimal control problem.

Contingent upon successful numerical simulations, I seek to implement this protocol in experiments at the Quantum Measurement and Control (QuMaC) Lab, TIFR Mumbai where I currently work under the supervision of Professor Rajamani Vijayaraghavan. A comparison of simulation and experimental performance would provide a complete picture of the efficacy of this application.

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