Quantum Optimal Control Theory

by

G.H. Gadiyar

Department of Mathematics, Indian Institute of Technology,
Madras 600 036, INDIA.

Abstract. The possibility of control of phenomena at microscopic level compatible with quantum mechanics and quantum field theory is outlined. The theory could be used in nanotechnology.
1. Motivation.

In technology physical processes are usually controlled by human intervention. The issue of finding the best in some sense or optimal control is an issue of great interest in a whole range of problems. These problems are also of interest to mathematicians. The classic solution to this problem was given by Pontryagin [1]. There have been many extensions and generalizations but for the extension of the theory to quantum phenomena the work of Pontryagin turns out to be the best. He has reduced the problem to one in the calculus of variations and completely solved the problem: the method is called the maximum principle.

The issue which will be addressed here is: How does one control quantum phenomena? At the level of quantum mechanics one has to respect the uncertainty principle and so the usual classical theory cannot be naively extended. At the level of quantum field theory one has to further respect the possibility of second quantization and creation of particles. It turns out that the difficulties can be side stepped and the quantum problems are almost as simple as the classical ones. Mathematical rigor is avoided: the pre-Weierstrass view that a physically sensible model possesses a mathematically sensible solution is taken. Rigorous proofs will be provided later.

The idea is to control microscopic phenomena. For example, can one minimize the time taken for a certain physical process? The hope is that in quantum computers with quantum switches, this theory can be applied to
optimize the time to switch from 0 to 1. It can also be used to invert the population in a laser in an optimal way. Such control is possible within the framework of the following theory.

2. The classical Pontryagin optimal control theory.

Consider any controlled process described by a system of ordinary differential equations

\[
\frac{dx_i}{dt} = f_i(x^1, ..., x^n; u^1, ..., u^r), \quad i = 1 \text{ to } n .
\]  

(1)

Here \(x^i\) are coordinates of the process (typically phase space coordinates.) and \(u^r\) are control parameters (usually external forces). For the process (1) to be defined

\[
u^j = u^j(t), \quad j = 1 \text{ to } r
\]  

(2)

are to be specified. Given

\[
x^i(t_0) = x^i_0, \quad i = 1 \text{ to } n ,
\]  

(3)

the solution to (1) is uniquely specified. Usually a functional

\[
J = \int_{t_0}^{t_1} f^0(x^1, ..., x^n; u^1, ..., u^r)dt
\]  

(4)

is to be optimized where \(f^0(x^n, u^r)\) is specified. If \(f^0(x^n, u^r) = 1\), \(J\) will be a time optimal problem.

The problem is to optimize (usually minimize) \(J\) by tuning the controls \(u^r\) such that the equations (1) are obeyed. Further in technical applications the
$u^r$ are usually constrained by the fact that the ‘forces’ cannot be arbitrarily large. Constraints like

$$|u^r| \leq C^r$$

are typical.

An example will fix the ideas: Consider a harmonic oscillator subject to a force. Bring it to rest in least time. Here the problem would be framed as

$$\frac{dx^1}{dt} = x^2$$
$$\frac{dx^2}{dt} = -x^1 + u, \quad |u| \leq 1$$

Here $x^1 = x$ is the position, $x^2 = p = \frac{dx}{dt}$ is the momentum and $u$ is the force. The functional $J = \int_{t_0}^{t_1} 1 \, dt$ is to be minimized.

The solution can be got by the Pontryagin principle but the physics of the solution can be seen as follows: The force $u$ should be applied always in the opposite direction to the velocity and should be of maximum magnitude. When the velocity changes sign the force jumps to the opposite direction again opposing the velocity. Thus the control jumps is piecewise continuous as a function of time. This is ‘bang-bang’ control as it is popularly called.

The theory of Pontryagin is summarized in the following results. Consider in addition to

$$\frac{dx^i}{dt} = f^i(x, u), \quad i = 1 \text{ to } n,$$

the equation

$$\frac{dx^0}{dt} = f^0(x, u)$$
coming from $J$, that is, now consider

$$\frac{dx^i}{dt} = f^i(x,u) \ , \ i = 0 \text{ to } n \ (\text{not } 1 \text{ to } n) .$$

Take an auxiliary set of variables $\psi_0 \text{ to } \psi_n$

$$\frac{d\psi_i}{dt} = -\sum_{\alpha=0}^{n} \frac{\partial f^\alpha}{\partial x^i} \psi_\alpha \ , \ i = 0 \text{ to } n .$$

This system is linear and homogeneous and we can combine the equations in to a Hamiltonian

$$\mathcal{H}(\psi, x, u) = \sum \psi_\alpha f^\alpha(x,u) ,$$

$$\frac{dx^i}{dt} = \frac{\partial \mathcal{H}}{\partial \psi_i} \ , \ i = 0 \text{ to } n ,$$

$$\frac{d\psi_i}{dt} = -\frac{\partial \mathcal{H}}{\partial x^i} \ , \ i = 0 \text{ to } n .$$

Denote by $\mathcal{M}(\psi, x) = \sup_{u \in U} \mathcal{H}(\psi, x, u)$ where we take the strict upper bound of $\mathcal{H}$ as a function of $u$ for given $\psi, x$.

**Theorem.** Let $u(t), t_0 \leq t \leq t_1$ be a permissible control. A necessary condition for $u(t)$ and $x(t)$ to be optimal is that there is a $\psi(t)$ corresponding to $x(t)$ so that

(1) given an $t_0 \leq t \leq t_1$

$$\mathcal{H}(\psi(t), x(t), u(t)) = \mathcal{M}(\psi(t), x(t)) , \quad (A)$$

that is $\mathcal{H}$ attains a maximum at $u(t)$.

(2) At the final instant $t_1$,

$$\psi_0(t_1) \leq 0 \ , \ \mathcal{M}(\psi(t_1), x(t_1)) = 0 . \quad (B)$$
Further if \( \psi(t), x(t) \) satisfy the equation of motion and \( |u(t)| \leq 1, \psi_0 \) and \( \mathcal{M}(\psi(t), x(t)) \) are constants and the equation (B) can be verified for all \( t, t_0 \leq t \leq 1 \) and not only at \( t_1 \).

**Example.**

\[
\mathcal{H} = \psi_1 x^2 - \psi_2 x^1 + \psi_2 u ,
\]

\[
\frac{dx^1}{dt} = x^2 , \quad \frac{dx^2}{dt} = -x^1 + u ,
\]

\[
\frac{d\psi_i}{dt} = \psi_2 , \quad \frac{d\psi_2}{dt} = -\psi_1 .
\]

So \( \psi_1 = A \sin(t - \alpha_0), A > 0 \) and \( \alpha_0 \) constant. Max \( \mathcal{H}(\psi, x, u) = \text{sign} \psi_2 = \text{sign}(A \sin(t - \alpha_0)) \). Hence the control is ‘bang-bang’ as intuitively argued earlier.

**3. Quantum mechanical controls.**

We cannot obviously generalize by replacing \( x \) and \( p \) by \( \hat{x} \) and \( \hat{p} \) or even \( \langle \hat{x} \rangle \) and \( \langle \hat{p} \rangle \) as a little thought will indicate. The way the problem is addressed is to consider the states \( |\phi> \) of the Schrödinger equation as the essential feature. What is meant is that the problem is now how does one optimally move a system from the initial state \( \phi_I \) to the final state \( \phi_F \) subject to some controls \( u_i \) and functional \( J = \int_{t_0}^t f^0(\phi, u)dt \).

Mathematically the problem is written as:

\[
\frac{i\hbar}{\partial t} \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} + V(x)\phi + u(x, t)\phi = \mathcal{H}_0\phi + u(x, t)\phi .
\]

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Here $u(x,t)$ is the controlling potential. The problem is to optimize some functional

$$ J = \int_{t_0}^{t_1} f^0(\phi, u) dt. $$

The answer to this problem now turns out to be very simple: it can be recast into a form where the Pontryagin principle can be applied. This is done as follows.

Consider $|n> as eigen functions of $H_0$,

$$ H_0|n> = E_n|n>. $$

Now

$$ i\hbar \frac{d\phi}{dt} = H\phi = (H + u(x,t))\phi $$

can be rewritten with $\phi(x,t) = \sum_{n=0}^{\infty} C_n(t)|n>$ as

$$ i\hbar \sum_{n=0}^{\infty} \dot{C}_n(t)|n> = H_0 \sum_{n=0}^{\infty} C_n(t)|n> + u(x,t) \sum_{n=0}^{\infty} C_n(t)|n>. $$

Now taking the inner product with $<m|, 

$$ i\hbar \sum_{n=0}^{\infty} \dot{C}_n(t) <m|n> = E_n C_n(t) <m|n> + C_n(t) <m|u|n> $$

$$ i\hbar \dot{C}_n(t) = C_n(t) + \sum_{m=0}^{\infty} u_{nm}(t) C_m(t). $$

This is now a linear system of ordinary differential equations and hence the Pontryagin theory can be applied! The technical problem is that the index $n$ runs from zero to infinity: that is a problem for mathematical analysts to
tackle. There is a simple case where we have a spin half particle: that is simpler and is a nice exercise to do.

4. Quantum field theory.

The same trick as the earlier section can be applied again! The procedure is as follows.

\[
[\phi(x), \phi(y)] = 0 ,
\]

\[
[\pi(x), \pi(y)] = 0 ,
\]

\[
[\phi(x), \pi(y)] = i \delta(x - y)
\]

are the canonical commutation relations. We can use a “Schrödinger picture”

\[
i \frac{\partial}{\partial t} \psi(\phi, t) = \mathcal{H}(-i \frac{\delta}{\delta \phi}, \phi) \psi(\phi, t)
\]

where \( \psi \) is a functional. Thus one can hope to extend the description of Section 3 to this situation as well. However two problems exist and have to be understood carefully. How to deal with Fermions and how to address renormalization effects. However in many body theory in condensed matter the method can be pushed through.

5. Conclusion.

The control problem and the Pontryagin principle can be easily extended to the quantum domain. Mathematically the problem is similar though questions of analysis (infinity and convergence) have to be addressed more carefully.
Technologically it is tempting to think of possible applications to

(1) laser population inversion

(2) quantum switching in quantum computers.

Reference.

[1] The mathematical theory of optimal processes, Pontryagin, Boltyanskii
Gamkrelidze and Mishchenko.