Control System Project

Optimal Quantum Control

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Abstract

In order to control the process of any quantum system, we need to obtain a control function that can control the process. In this report, we explain a method/process called "Optimal Control Function" to try and achieve the same.

Introduction and the need for quantum control systems

A major problem in all the quantum systems is that they are very sensitive to the presence of environment which often destroys the main features of quantum dynamics. This is known as de-coherence. Quantum decoherence in physics and quantum computing is the loss of quantum coherence. Quantum coherence is the idea that an individual particle or object has wave functions that can be split into two separate waves. Quantum decoherence happens when there is no longer a definite phase relation between the two different states. When the waves operate together in a coherent way, that's referred to as quantum coherence. Decoherence also explains within quantum theory why macroscopic objects seem to possess their familiar classical properties.

This is where the role of quantum control systems kicks in. One method to prevent de-coherence is to obtain the desired state transfer in the least possible time so that the interaction with the environment becomes negligible. The treatment of the time optimal control problem uses different tools depending on whether or not there is a prescribed bound on the control magnitude. For unbounded controls, the time optimal control does not exist.

What is optimal Control?

In many experimental setups, an electromagnetic field interacts with a system, whose dynamics follows the laws of quantum mechanics. While it is appropriate to treat the latter system as a quantum mechanical one, the electromagnetic field can often be treated as a classical field, giving predictions that agree with macroscopic observation.

This is the so-called semi-classical approximation. With technological advances of the last decades, it is now possible to shape the interacting electromagnetic field almost at will. This leads to a point of view which considers these experiments as control experiments where the electromagnetic field plays the role of the control and any other quantum mechanical system, in this case is the object of the control.

We will address the problem of optimal control and formulate optimal control function in the next sections.

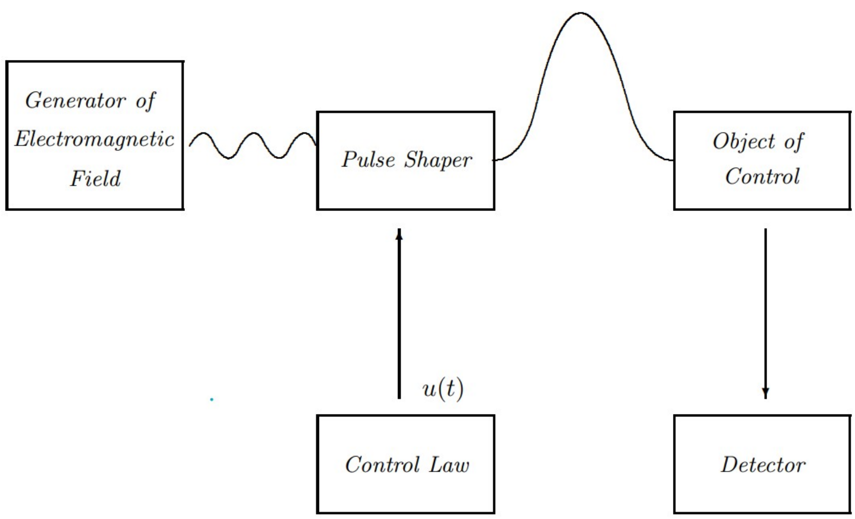

Figure 1: Quantum Control experiment scheme

Formulation of the Optimal Control Problem

Given a set X of (state) functions x: R $\rightarrow$ R^n, and a set U of (control) functions u : R $\rightarrow$ R^m, find functions $x \in X$ and $u \in U$ which minimize a cost functional $J : X \times U \rightarrow R$

Say that we want to find a piece wise continuous control u to drive the state x from a given value x_0 to a final value x_f in time T. Then U is the set of piece wise continuous functions on [0, T], X can be taken as the set of continuous functions on [0, T]. Thus the cost function we need to minimize can be given by:

$$J(u) = ||x(T) - x_f||^2 \tag{1}$$

which is nothing but the euclidean distance between the final and desired state values. We can also incorporate a term that considers the energy used during a given interval of time. For example, in the form below $\lambda > 0$, will introduce a penalty on the final state and and energy like term for the control.

$$J(u) = \lambda ||x(T) - x_f||^2 + \int_0^T ||u(t)||^2 dt \tag{2}$$

We can thus manipulate the value of λ to control the amount of energy used to obtain a more accurate final state.

Different formulations of optimal control problems

1. Problem of Mayer:

The problem of Mayer is to determine a control function u, in an appropriate set of functions, to minimize the cost functional in the form

$$J(u) = \phi(x(T), T) \tag{3}$$

where ϕ is a smooth function. In mathematical analysis, the smoothness of a function is a property measured by the number of continuous derivatives it has over some domain, called differentiability class. At the very minimum, a function could be considered smooth if it is differentiable everywhere (hence continuous). At the other end, it might also possess derivatives of all orders in its domain, in which case it is said to be infinitely differentiable and referred to as a C-infinity function. Mayer problems arise when there is a particular emphasis on the final state and/or time.

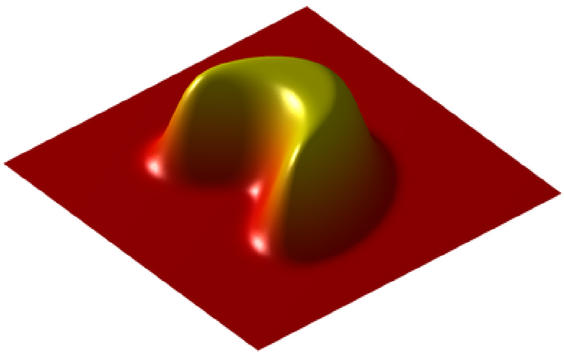

Figure 2: Bump function as an example of a smooth function(has continuous derivatives of all orders)

2. Problem of Lagrange:

In the problem of Lagrange, the cost functional takes the form:

$$J(u) = \int_0^T L(x(t), u(t), t)dt \tag{4}$$

where L is a smooth function. This problem occurs when the cost accumulates with time. For example, it can be used to minimize the energy used in the time duration required to reach the final state.

3. Problem of Bolza:

The problem of Bolza is a combination of the problems of Mayer and Lagrange as the cost takes the form:

$$J(u) = \phi(x(T), T) + \int_0^T L(x(t), u(t), t)dt \tag{5}$$

where ϕ and L are smooth functions. Bolza problem arises when when there is a cumulative cost which increases during the control action but special emphasis is placed on the situation at the final time.

Optimal control problems for quantum systems

For further discussion, to avoid complex mathematics we will consider the state (x) to be a pure state. The dynamics of a quantum system is described by the Schrödinger equation:

$$\frac{d}{dt}\overrightarrow{\psi} = -iH(u)\overrightarrow{\psi} \tag{6}$$

The general Bolza type cost function is given as:

$$J(u) = \phi(\overrightarrow{\psi}(T), T) + \int_0^T L(\overrightarrow{\psi}(t), u(t), t)dt \tag{7}$$

Now, both $\overrightarrow{\psi}$ and matrix $-iH(u)$ are complex. To express them in real quantities, we can write:

$$\overrightarrow{\psi} = \overrightarrow{\psi}_R + i\overrightarrow{\psi}_I \tag{8}$$

$$-iH(u) = R(u) + iI(u) \tag{9}$$

Here R(u) and I(u) are real n × n matrix functions of u, R(u) skew-symmetric and I(u) symmetric for every value of u. Now using the above equations and the Schrödinger equation we get two real differential equations:

$$\frac{d}{dt}\overrightarrow{\psi}_R = R(u)\overrightarrow{\psi}_R - I(u)\overrightarrow{\psi}_I \tag{10}$$

$$\frac{d}{dt}\overrightarrow{\psi}_I = I(u)\overrightarrow{\psi}_R - R(u)\overrightarrow{\psi}_I \tag{11}$$

Say,

$$x := [\overrightarrow{\psi}_R^T \overrightarrow{\psi}_I^T]^T \tag{12}$$

$$\tilde{H}(u) = \begin{bmatrix} R(u) & -I(u) \\ I(u) & R(u) \end{bmatrix} \tag{13}$$

We can thus write the differential equation describing the dynamics involving only real quantities as:

$$\dot{x} = \tilde{H}(u)x \tag{14}$$

Also the cost function can thus be written as:

$$J(u) = \tilde{\phi}(x(T), T) + \int_0^T \tilde{L}(x(t), u(t), t)dt \tag{15}$$

Necessary Conditions for Optimal Control

A control function is considered optimal when its cost function is the least. Putting it in mathematical terms, assume there exists a condition u^ϵ that differs slightly from the optimal condition u, then the corresponding cost functions should be such that,

$$J(u^\epsilon) - J(u) > 0 \tag{16}$$

From the image below, we can see that the third image is a slight modification of the optimal control function whereas the second image differs wildly from the optimal control function. Therefore, the cost function of the optimal condition should always be the least.

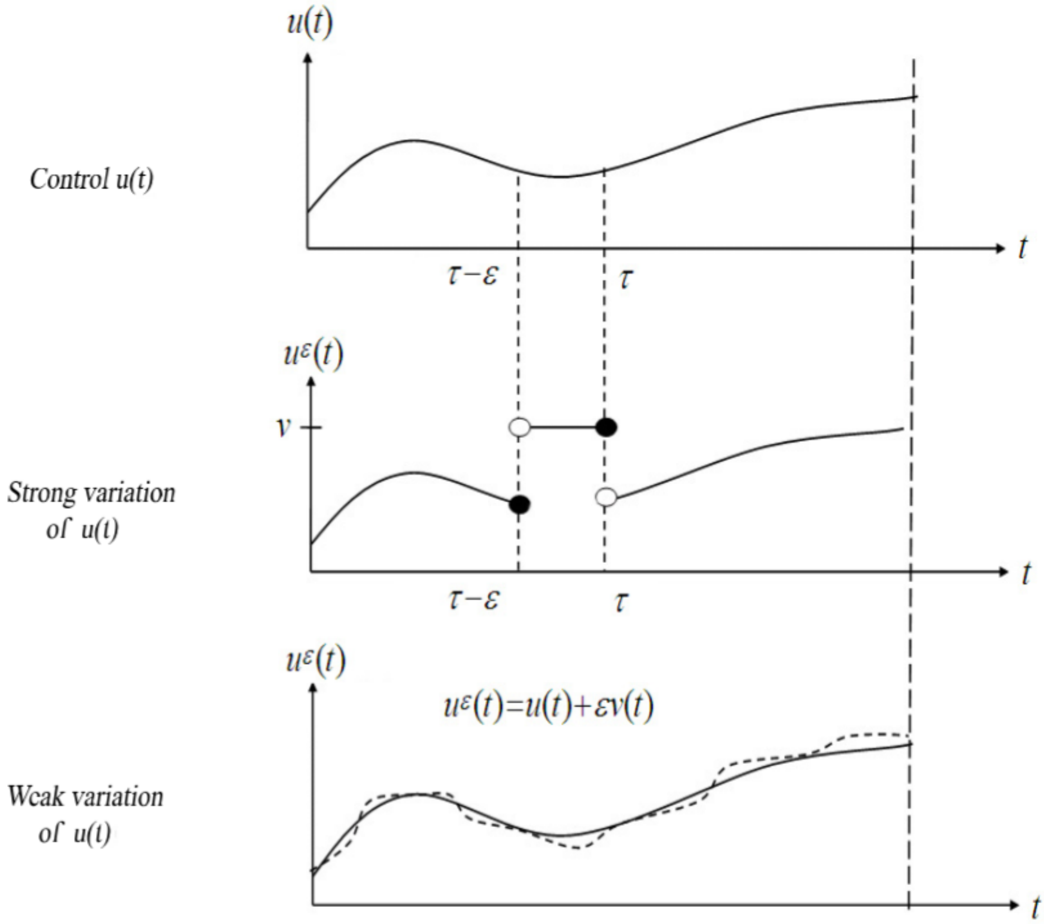

Figure 3: The Various types of modifications.

In order to obtain said cost function and enforce the necessary condition, there exists a theorem called Pontryagin maximum principle. It is defined as follows:-

Assume u is the optimal control and x is the corresponding trajectory solution (i.e., state variable). Then, there exists a nonzero vector λ solution of the adjoint equations

$$\dot{\lambda}^T = -\lambda^T f_x(x(t), u(t)) \tag{17}$$

with terminal condition:

$$\lambda^T(\tau) = -\phi_x(x(\tau)) \tag{18}$$

such that, for every $\tau \in (0, T]$, we have :

$$\lambda^T(\tau) f(x(\tau), u(\tau)) \geq \lambda^T(\tau) f(x(\tau), v) \tag{19}$$

for every v in the set of admissible values for the control U. Here the λ is called the co-state matrix. In order to simplify calculations further one uses the The Pontryagin maximum principle in the following way. One defines a function:-

$$h = h(\lambda, x, u) := \lambda^T f(x, u) \tag{20}$$

This function is also called as the "optimal control Hamiltonian". For every λ and x,one maximizes this function over $u \in U$, i.e., u is chosen so that for every λ and x,

$$h(\lambda, x, u) \geq h(\lambda, x, v) \tag{21}$$

After finding the control function u with respect to these parameters λ and x, we can further optimize it by changing the respective values of λ and x. The solution will depend on these parameters and we can write it as u := u(x, λ).

Now in order to obtain the control equation we can solve the above with the help of the conditions we initially took, that is,

$$\dot{x} = f(x, u(x, \lambda)), \tag{22}$$

and also the adjoint equation from the Pontryagin maximum principle.

$$\lambda^T(\tau) f(x(\tau), u(\tau)) \geq \lambda^T(\tau) f(x(\tau), v) \tag{23}$$

From the above two equations we get equations that can be solved using the boundary conditions.

$$x(0) = x_0 \tag{24}$$

$$\lambda^T(T) = -\phi_x(x(T)) \tag{25}$$

The above boundary condition is a two points boundary value problem as the boundary conditions are at time 0 and T. By simplifying the equations, we finally get $\lambda(0)$, as a free parameter, which we then try to adjust to accommodate the final condition mentioned in the Pontryagin maximum principle i.e. equation (8). Every control which satisfies the necessary optimality conditions is called an extremal. As mentioned before, after obtaining the control function with respect to the parameters, we can adjust it to find various control function and the one with the least cost is the optimal control function. The above problem is for a mayer problem.

If we encounter a Bolza problem, we can easily adapt the entire thing for the same. We start by defining an extra variable:-

$$y(t) := \int_0^T L(x(s), u(s), s)\, ds \tag{26}$$

We then redefine the existing cost function:-

$$J(u) := \phi(x(T)) + \int_0^T L(x(s), u(s), s)\, ds \tag{27}$$

In the form of the Mayer cost function:-

$$J(u) = \bar{\phi}(x(T), y(T)) = \phi(x(T)) + y(T). \tag{28}$$

The co-state now has dimension n +1. If we call λ the first n components of the costate and μ the remaining component, the adjoint equations take the form

$$\dot{\lambda}^T = -\lambda^T f_x - \mu L_x, \dot{\mu} = 0. \tag{29}$$

So μ is a constant, and since $\mu(T) = -\phi_y = -1$, we have that condition (21) can be rewritten with the Hamiltonian

$$h(\lambda, x, u) = \lambda^T f(x, u) - L(x, u). \tag{30}$$

Hence, we can say that for a Bolza problem, with fixed final time and free final state, if u is optimal, then it satisfies (21) with h given in (28). λ satisfies the first of (27) with terminal boundary condition and the conditions mentioned previously.

Optimal Conditions for a quantum system

We know that the for a quantum system, we can define the system as:-

$$\dot{x} = \tilde{H}(u)x \tag{31}$$

From equation (28) shown in the previous section, we can say that the optimal control hamiltonian takes the following form:-

$$h(\lambda, x, u) = \lambda^T \tilde{H}(u)x - \tilde{L}(x, u). \tag{32}$$

The optimal control u has to satisfy (21) with this Hamiltonian. The adjoint equations are

$$\dot{\lambda}^T = \lambda^T \tilde{H}(u)x + \tilde{L}_x. \tag{33}$$

Since $\tilde{H}(u)$is skew-symmetric, can be written as

$$\dot{\lambda} = \tilde{H}(u)\lambda + \tilde{L}_x^T. \tag{34}$$

and the terminal condition are same as before.

From the above equations we can say that if the cost does not depend on the state x, then the differential of the cost w.r.t x will be zero which would render the above equation as:-

$$\dot{\lambda} = \tilde{H}(u)\lambda \tag{35}$$

This would mean that λ and x satisfy the same equations and conditions. We can leverage this property to solve many problems. This would also mean that λ and x are coupled only through the controls

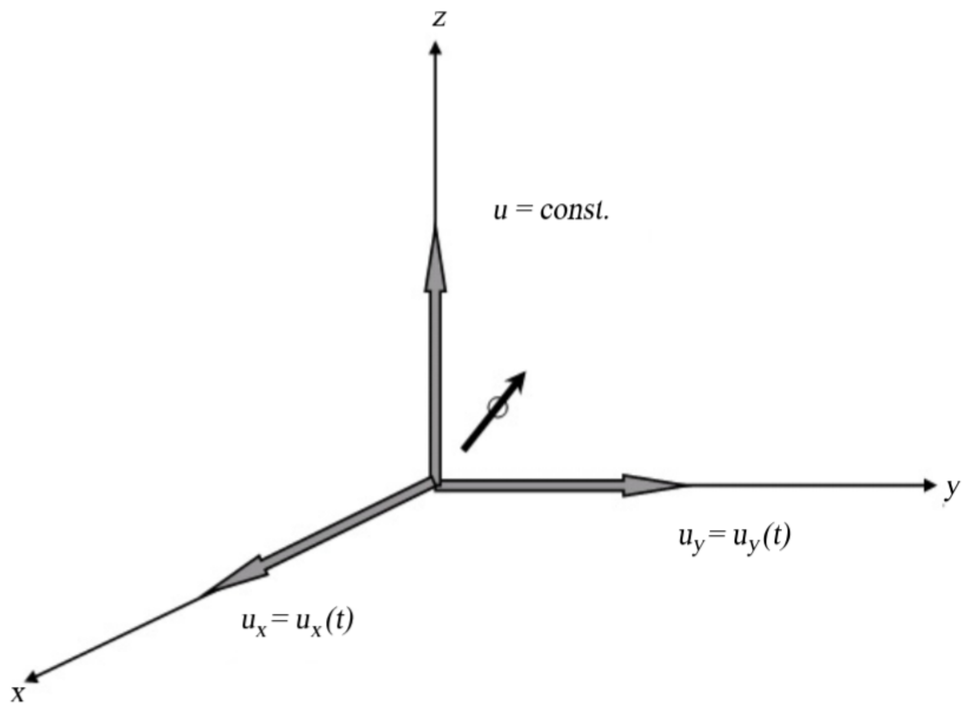

Figure 4: Field in various directions.

Example Problem to find Optimal Control

Spin is an intrinsic property of any particle. We can control the spin of any particle with the help of electro-magnetic field.

Let us take the example of a particle which has a spin of $+\frac{1}{2}$ initially in the presence of an external electromagnetic field:-

$$\dot{\phi} = (\bar{\sigma}_z u_z + \bar{\sigma}_x u_x + \bar{\sigma}_y u_y)\phi \tag{36}$$

where,

$$\bar{\sigma}_z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{37}$$

$$\bar{\sigma}_x = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

$$\bar{\sigma}_y = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For ease of calculation and understanding, we assume the field component in the z axis to be constant.

Since ϕ describes the state of the system, we can replace ϕ with a more generic term x, the state variable to prevent confusion.

$$\dot{x} = (\bar{\sigma}_z u_z + \bar{\sigma}_x u_x(t) + \bar{\sigma}_y u_y(t))x \tag{38}$$

We observe that the above equation is analogous to that of a quantum system, where:-

$$\tilde{H}(u) = (\bar{\sigma}_z u_z + \bar{\sigma}_x u_x(t) + \bar{\sigma}_y u_y(t)) \tag{39}$$

which would then become:-

$$\dot{x} = \tilde{H}(u)x \tag{40}$$

Now consider the cost function for the above differential equation:-

$$J(u_x, u_y) = -Re(\vec{\phi}^T(T)\vec{\phi}_f) + \eta \int_T^0 u_x^2(t) + u_y^2(t)/, dt \tag{41}$$

In order to get the real component for the cost function, we can modify the differential equation to obtain its real components:-

$$\dot{x} = (\bar{T}_z u_z + \bar{T}_x u_x(t) + \bar{T}_y u_y(t))x \tag{42}$$

where,

$$\bar{T}_x = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{43}$$

$$\bar{T}_y = \frac{1}{2}\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\bar{T}_z = \frac{1}{2}\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

We can observe that the above equations commutation relations

$$[T_x, T_y] = T_z \tag{44}$$

$$[T_y, T_z] = T_x$$

$$[T_x, T_z] = T_y$$

The cost function can be re-written as:-

$$J(u_x, u_y) = -x^T(T)x_f + \eta \int_T^0 u_x^2(t) + u_y^2(t)/, dt \tag{45}$$

From the above, we can observe that the integral function is independent of x. Invoking the property mentione before we can see that the co-state satisfies the same equations as x.

$$\dot{\lambda} = (\bar{T}_z u_z + \bar{T}_x u_x(t) + \bar{T}_y u_y(t))\lambda \tag{46}$$

The optimal control hamiltonian is obtained as:-

$$h(\lambda, x, u_x, u_y) = \lambda^T(\bar{T}_z u_z + \bar{T}_x u_x(t) + \bar{T}_y u_y(t))x - \eta(u_x^2 + u_y^2) \tag{47}$$

As we know that the optimal function is the extremal, we can obtain those conditions by differentiating the above equations from which we get:-

$$u_x = \frac{1}{2\eta}\lambda^T T_x x \tag{48}$$

$$u_y = \frac{1}{2\eta}\lambda^T T_y y$$

Using the original quantum state equation, commutative property and differentiating the above equations again we get that:-

$$\dot{u}_x = \frac{1}{2\eta}(\lambda^T T_z x u_y - u_z u_y) \tag{49}$$

$$\dot{u}_y = \frac{1}{2\eta}(\lambda^T T_z x u_x - u_z u_x)$$

$$\frac{d}{dt}\lambda^T T_z x = 0 \tag{50}$$

From the above three equations we get that,

$$\dot{u}_x = k u_y \tag{51}$$

$$\dot{u}_y = k u_x$$

where $k = \frac{1}{2\eta}(\lambda^T T_z x - u_z)$ is a constant. By solving the equations we get that,

$$u_x(t) = M \cos \omega t + \gamma$$

$$u_y(t) = M \sin \omega t + \gamma$$

We can further lower the cost of by changing the values of M, ω, γ.

Conclusion

In conclusion, the Pontryagin maximum principle allows to transform an infinite dimensional optimization problem (the search over a set of functions) into a finite dimensional optimization problem (the search over a set of parameters). We can obtain the optimal control functions for many quantum problems.