Time Scaling Transformation in Quantum Optimal Control Computation

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Outline

Introduction

Quantum Optimal Control is widely used in the quantum systems:

- Superconducting quantum systems
- Nuclear magnetic resonance (NMR)
- Bose-Einstein condensates

Many methods have been developed for the closed quantum systems:

- Gradient Method: GRadient Ascent Pulse Engineering (GRAPE, Khaneja); Krotov Method
- Geometric Method: Quantum Brachistochrone Equation (QBE, Carlini); Geodesic Equation (Nielsen)
- Others: Pseudospectral Method; Dynamic Programming

Outline

Problem Formulation

According to the Schrödinger equation, the closed quantum systems can be formulated as the bilinear control systems in the absence of relaxation.

$$\dot{U}(t) = -i\left(H_d + \sum_{l=1}^{m} u_l(t)H_l\right)U(t)$$

Given evolutionary time T, the goal is to drive the system to implement the designated quantum gate U_f within admissible control (due to the physical constraints).

$$\begin{aligned}&\max J(\boldsymbol{u}(t)) = 2^{-N}\Re(tr\{U_f^\dagger U(T)\}), \boldsymbol{u}(t) = [u_1(t), u_2(t), \cdots, u_m(t)]\\ &s.t. \, |u_l(t)| \leq u_{l\,\max}, \forall l = 1, 2, \cdots, m\end{aligned}$$

Outline

Piecewise-Constant Parameterization

The continuous control can be discretized by the approximation:

$$u(t) \approx u^M(t) = \sum_{k=1}^{M} \sigma^k \chi_{[t_{k-1},t_k)}(t)$$

$$\chi_{[t_{k-1},t_k)}(t) = \begin{cases} 1, \text{if } t \in [t_{k-1}, t_k) \\ 0, \text{otherwise} \end{cases}$$

$$0 = t_0 < t_1 < \cdots < t_{M-1} < t_M = T$$

The parameterized Schrödinger equation is shown below:

$$\dot{U}(t) = \sum_{k=1}^{M} -i \left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l \right) U(t) \chi_{[t_{k-1},t_k)}$$

$$U(0) = I_{2^N \times 2^N}$$

Piecewise-Constant Parameterization

The solution can be expressed as $U(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu})$, where

$$\boldsymbol{\sigma} = [\boldsymbol{\sigma}^{\mathbf{1}}; \boldsymbol{\sigma}^{\mathbf{2}}; \cdots; \boldsymbol{\sigma}^{\boldsymbol{M}}] \in \mathbb{R}^{Mm}; \boldsymbol{\sigma}^{\boldsymbol{k}} = [\sigma_1^k, \sigma_2^k, \cdots, \sigma_m^k]^{\mathrm{T}}$$
$$s.t. \left|\sigma_l^k\right| \leq \sigma_{l\max}, \forall l = 1, 2, \cdots, m, \forall k = 1, 2, \cdots, M$$
$$\boldsymbol{\nu} = [t_1, \cdots, t_{M-1}] \in \mathbb{R}^{M-1}$$
$$s.t. 0 = t_0 < t_1 < \cdots < t_{M-1} < t_M = T$$

The objective function of parameterized Schrödinger equation is shown below:

$$J(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu}) = 2^{-N}\Re(tr\{U_f^\dagger U(T)\})$$
$$= 2^{-N}\Re(tr\{U_f^\dagger U_M(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu}) U_{M-1}(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu}) \cdots U_1(\cdot|\boldsymbol{\sigma}, \boldsymbol{\nu})\})$$

Time Scaling Transformation

New time variable and time-related decision parameters are introduced respectively as $s \in [0, M]$ and

$$\boldsymbol{\theta} = [\theta_1, \theta_2, \cdots, \theta_M], \quad \theta_k = t_k - t_{k-1}, \forall k = 1, 2, \cdots, M$$

$$s.t.\ \theta_k \geq 0, \sum_{k=1}^{M} \theta_i = T$$

where $t(s) = \theta_k \cdot s, s \in [k-1, k), \forall k = 1, 2, \cdots, M$ Hence, the original Schrödinger equation can be written as:

$$\dot{\tilde{U}}(s) = -i \left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l \right) \tilde{U}(s)\theta_k$$

$$\tilde{U}(0) = I_{2^N \times 2^N}, \quad s \in [k-1, k), \forall k = 1, 2, \cdots, M$$

Gradient Ascent Pulse Engineering

On the assumption that θ_k is small enough, or rather

$$\theta_k \ll \left\| H_d + \sum_{l=1}^{m} \sigma_l^k H_l \right\|^{-1}$$

As calculating accurate gradient is very time-consuming, the gradients of evolutionary matrix over the control can be approximated:

$$\begin{aligned}
\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k} &\approx -i\theta_k H_l U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu}) \\
\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k} &= -i\left(H_d + \sum_{l=1}^{m} \sigma_l^k H_l\right) U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu}) \\
\frac{\partial J(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k} &= 2^{-N}\Re(tr\{\Lambda_{M+1:j+1}^{\dagger}\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \sigma_l^k}X_{j-1:0}\}) \\
\frac{\partial J(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k} &= 2^{-N}\Re(tr\{\Lambda_{M+1:j+1}^{\dagger}\frac{\partial U_k(\cdot|\boldsymbol{\sigma},\boldsymbol{\nu})}{\partial \theta_k}X_{j-1:0}\})
\end{aligned} \tag{1}$$

The improved GRAPE algorithm (with time scaling transformation) follows :

1) Initialize the counters.
2) Outer loop: Initialize $\boldsymbol{\sigma}, \boldsymbol{\nu}$ randomly within admissible sets.
3) Inner loop: Given initial control parameters, calculate the exponent, forward propagation, backward propagation, and the objective function, or fidelity as below.

$$
\begin{aligned}
X_{j:0} &= U_j U_{j-1}, \cdots, U_2 U_1 \\
\Lambda^{\dagger}_{M+1:j+1} &= U_f^{\dagger} U_M U_{M-1}, \cdots U_{j+1} \\
\Phi &= 2^{-N} \Re\{tr(\Lambda^{\dagger}_{M+1:j+1} X_{j:0})\}
\end{aligned}
$$

4) If target fidelity is not reached, update the control parameters according to the gradients as formula (1) or the exact gradients. Other options are numerical gradients including Newton, Quasi-Newton, L-BFGS, etc.
5) If target fidelity is still not reached after multiple iterations, finish the inner loop, then choose another initial guess of parameters and restart the inner loop.
6) If target fidelity is reached, finish the outer loop, and smooth the pulse

Outline

Optimal Control for the Homonuclear Spins

Then the homonuclear spins in the liquid nuclear magnetic resonance (*lNMR*) can be formulated in the rotating frame as

$$\dot{U}(t) = -i\left(H_Z + H_J + H_{RF}\right)U(t)$$

$$H_z = -\sum_{i=1}^{N}[(1-\delta_i)\omega_0 - \omega_{rf}]S_z^{\otimes i}$$

$$H_J = 2\pi J_{ij}\sum_{i<j}(S_x^i S_x^j + S_y^i S_y^j + S_z^i S_z^j)^{\otimes}$$

$$H_{RF} = -\sum_{i=1}^{N}(1-\delta_i)[u_x(t)S_x^{\otimes i} - u_y(t)S_y^{\otimes i}]$$

The two quantum bits system is control by the 2-channels radio frequency magnetic field marked as x and y.

Optimal Control for the Homonuclear Spins

Taking for example the 4^{th} and 5^{th} carbon atoms in the L-Histidine molecule in Fig. 1. Set the target quantum gate to be $R_x(\pi/2) \otimes I_{2\times 2}$

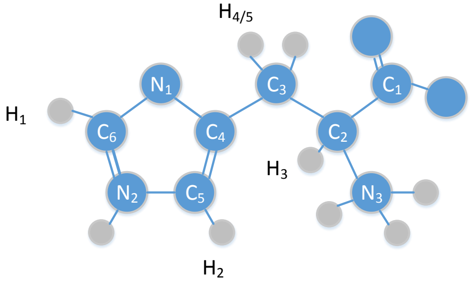

Figure 1: L-Histidine Structure Diagram.

Numerical Simulation

Their chemical shifts are respectively $\delta_1\omega = -22562Hz$ and $\delta_2\omega = -20657Hz$ under the $600MHz$ NMR. The simulation parameters are:

$$N = 2, m = 2, M = 50, \omega = 150MHz, \delta_1\omega = -22562Hz,$$
$$\delta_2\omega = -20657Hz, \sqrt{u_x^2 + u_y^2} \leq \Omega_{\max} = 12.5kHz$$

Where maximum control power is $\Omega_{\max}$. The minimum can be estimated by the geodesic distant:

$$T_{\mathrm{minimum}} \gtrsim T_{\mathrm{geodesic}} = \frac{\left\| \log(U_{1f}^{\dagger} U_{2f}) \right\|}{\|(\delta_1 - \delta_2)\omega_0 S_z\|} = 132\mu s$$

Numerical Simulation I

If $T = 150\mu s > T_{\text{minimum}}$, high fidelity $1 - 5.95078 \times 10^{-5}$ can be reached.

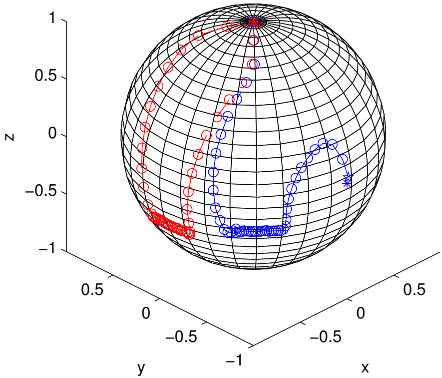

Figure 2: The blue line denotes the evolution of the first bit on the Bloch sphere, while the red line denotes the second bit.

Numerical Simulation II

If $T = 120\mu s < T_{\mathrm{minimum}}$, the fidelity cannot reach 1 theoretically.

Table 1: Simulation Results

No.	Algorithm	Fidelity	No. of Parameters
$T = 120\mu s < T_{\mathrm{minimum}}$			
1	Initial Sequence	0.9747153	100
2	M=75 GRAPE	0.9748384	150
3	M=100 GRAPE	0.9749424	200
4	M=50 Time Scaling	0.9749855	150
$T = 150\mu s > T_{\mathrm{minimum}}$			
5	Initial Sequence	0.9999405	100

Numerical Simulation II

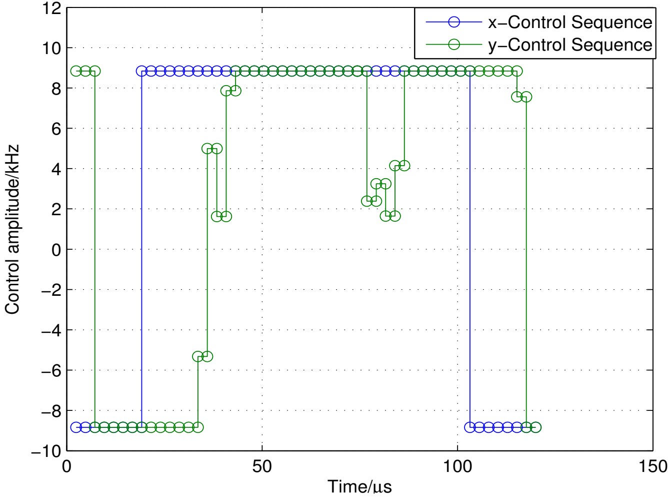

Figure 3: Control Sequence of Simulation 1. Time horizon is uniformly divided.

Numerical Simulation II

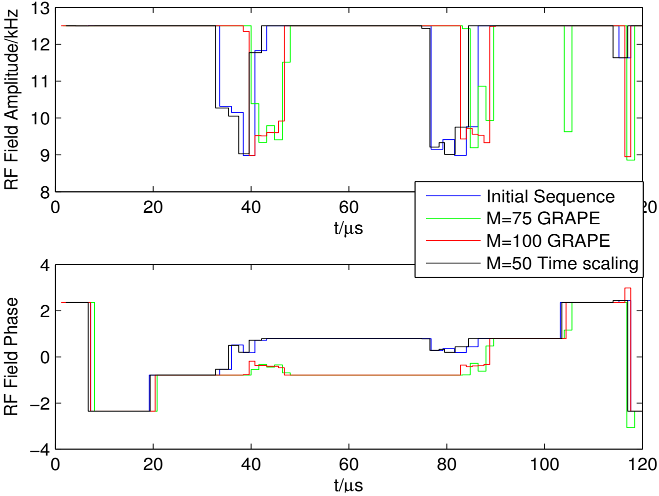

Figure 4: The amplitudes and phases of four simulations, the black one has the maximum fidelity. Plotted in stairs.

Numerical Simulation II

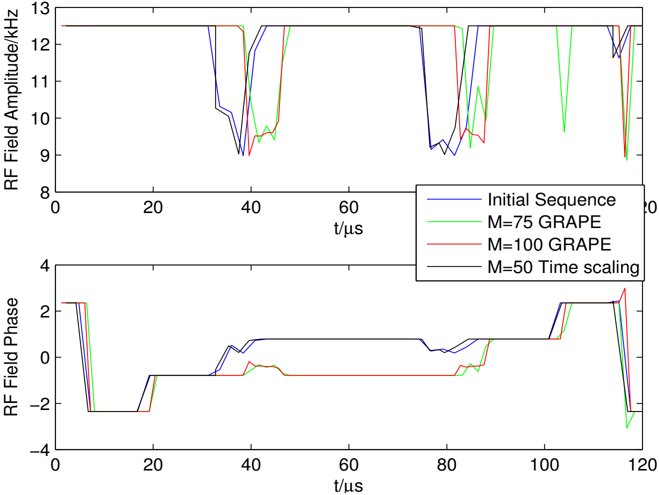

Figure 5: The amplitudes and phases of four simulations, the black one has the maximum fidelity.

Numerical Simulation II

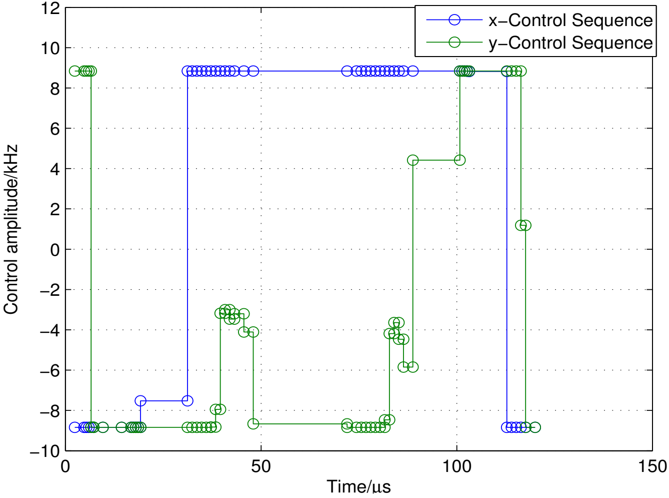

Figure 6: Control Sequence of Simulation 4. Time horizon is manually designated.

Error Reduction

The actual pulse can only be implemented with trailing edge. The actual pulse can be modeled as the step response of a 2^{nd}-order filter. The error is calculated as below, where ς is between 0 and 1, related to the response speed and overshoot.

$$e(t) = -e^{-\varsigma t/T} \sin(t\sqrt{1-\varsigma^2}/T + \arctan\sqrt{1-\varsigma^2})$$

This error can be proved to reduce when the time horizon of the rising or decline part is subdivided into more segments. The switching points on the time horizon can be adjusted to be concentrated when the pulse has a dramatic variation, and vice versa. The swithing points can be mannuly arbitrarily designated as shown in Fig. 6.

Outline

Conclusion

- The gradient method with time scaling transformation is proposed.
- Strengths: higher fidelity; fewer parameters; error reduction; arbitrarily set switching points.
- Drawbacks: Arbitrary fractional switching times are hard to implement in reality.

- future
  - Comparison experiment
  - Hardware nonlinearity

Major References I

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