Sampling-based learning control of inhomogeneous quantum ensembles

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Compensation for parameter dispersion is a significant challenge for control of inhomogeneous quantum ensembles. In this paper, we present a systematic methodology of sampling-based learning control (SLC) for simultaneously steering the members of inhomogeneous quantum ensembles to the same desired state. The SLC method is employed for optimal control of the state-to-state transition probability for inhomogeneous quantum ensembles of spins as well as Λ type atomic systems. The procedure involves the steps of (i) training and (ii) testing. In the training step, a generalized system is constructed by sampling members according to the distribution of inhomogeneous parameters drawn from the ensemble. A gradient flow based learning and optimization algorithm is adopted to find the control for the generalized system. In the process of testing, a number of additional ensemble members are randomly selected to evaluate the control performance. Numerical results are presented showing the success of the SLC method.

I. INTRODUCTION

Control of quantum phenomena lies at the heart of emerging quantum technology [1]-[4]. Quantum control theory has many components including controllability assessment, optimal control, feedback control, etc. Most existing results focus on control design of single quantum systems [1]-[18]. Another important issue is control design for quantum ensembles. A quantum ensemble consists of a large number of (up to ~10^20) single quantum systems (e.g., spin systems) and every quantum system is referred to as a member of the ensemble in this paper. Quantum ensembles have wide applications in emerging quantum technology including quantum computation [19], long-distance quantum communication [20], quantum memory [21], and magnetic resonance imaging [22]. Several results on quantum ensemble control have been presented including unitary control in homogeneous quantum ensembles for maximizing signal intensity in coherent spectroscopy [23] and feedback stabilization of quantum ensembles [24].

In practical applications, the members of a quantum ensemble could have variations in the parameters that characterize the system dynamics [25], [26]. For example, the spins of an ensemble in nuclear magnetic resonance (NMR) experiments may encounter large dispersion in the strength of the applied radio frequency field (rf inhomogeneity) as well as the members exhibiting variations in their natural frequencies (Larmor dispersion) [27], [28]. In this paper, these situations are referred as inhomogeneous quantum ensembles. It is generally impractical to employ different control inputs for individual members of a quantum ensemble in the laboratory. Hence, it is important to develop the means for designing control fields that can simultaneously steer the ensemble of systems from an initial state to a desired target state when variations exist in the system parameters. Such controls are also called compensating pulse sequences in NMR spectroscopy [25], [29]. Other applications include control of a randomly oriented ensemble of molecules in physical chemistry [30], the design of slice selective excitation and inversion pulses in magnetic resonance imaging, and the correction of systematic errors in quantum information processing [26]. Theoretical results showed that under commonly arising conditions there exist optimal laser fields to control all molecules in an inhomogeneous ensemble, regardless of their orientation or spatial location [31], [32]. Recent studies considered the controllability and optimal control of inhomogeneous spin ensembles [22], [26], [33]-[36]. An additional investigation considered the stabilization of an inhomogeneous ensemble of non-interacting spin systems using Lyapunov control methodology [37].

This paper presents a systematic methodology for control design of inhomogeneous quantum ensembles for the state-to-state transition probability, specifically for spins and three-level Λ type systems. The proposed method involves the steps of (i) training and (ii) testing, and we call sampling-based learning control (SLC). In the training step, we sample several members according to the distribution of inhomogeneous learning control parameters from the ensemble and construct a generalized system using these collective samples. Then we employ a gradient flow based learning and optimization algorithm [38] to find the control providing good performance for the generalized system. In the process of testing the deduced controls, we randomly select a number of sampling members to evaluate the control performance. Numerical simulations show that the
SLC method has potential for practical control design of various inhomogeneous quantum ensembles. These findings support the previous theoretical analysis suggesting that control on inhomogeneous ensembles should generally be feasible.

The paper is organized as follows. Section II formulates the control problem for inhomogeneous quantum ensembles and presents the details of SLC. The SLC method is illustrated for a two-level inhomogeneous quantum ensemble in Section III, and for a three-level inhomogeneous quantum ensemble in Section IV. Conclusions are presented in Section V.

II. METHODOLOGY

A. Model and problem formulation

Consider a finite-dimensional closed quantum system where the evolution of its state $|\psi(t)\rangle$ is described by the Schrödinger equation (setting $h = 1$):

$$
\begin{align*}
\frac{d}{dt}|\psi(t)\rangle &= -iH(t)|\psi(t)\rangle, \\
&\quad t \in [0, T], \quad |\psi(0)\rangle = |\psi_0\rangle.
\end{align*}
$$

The solution of (1) is given by $|\psi(t)\rangle = U(t)|\psi_0\rangle$, where the propagator $U(t)$ satisfies

$$
\begin{align*}
\frac{d}{dt}U(t) &= -iH(t)U(t), \\
&\quad t \in [0, T], \quad U(0) = \text{Id}.
\end{align*}
$$

In this paper, we consider an inhomogeneous ensemble in which the Hamiltonian of each member has the following form

$$
H_{\omega, \theta}(t) = g(\omega)H_0 + b(\theta) \sum_{m=1}^{M} u_m(t)H_m,
$$

where $H_0$ is the free Hamiltonian and $\sum_{m=1}^{M} u_m(t)H_m$ corresponds to the time-dependent control Hamiltonian that represents the interaction of the system with the external fields $u_m(t)$ (real-valued and square-integrable functions) through Hermitian operators $H_m$. The functions $g(\omega)$ and $b(\theta)$ characterize the inhomogeneous distribution in the free Hamiltonian and control Hamiltonian, respectively (see Fig. 1). In this paper, we assume that $g(\omega) = \omega$ and $b(\theta) = \theta$, and the parameters $\omega$ and $\theta$ are time independent and uniformly distributed over $[1 - \Omega, 1 + \Omega]$ and $[1 - \Theta, 1 + \Theta]$, respectively. The constants $\Omega \in [0, 1]$ and $\Theta \in [0, 1]$ represent the bounds of the parameter dispersion. The objective is to design the controls $\{u_m(t), m = 1, 2, \ldots, M\}$ to simultaneously drive the members (with different $\omega$ and $\theta$) of the quantum ensemble from an initial state $|\psi_0\rangle$ to the same target state $|\psi_{\text{target}}\rangle$ with high fidelity. The control outcome is described by a performance function $J(u)$ for each control strategy $u = \{u_m(t), m = 1, 2, \ldots, M\}$. The control problem can then be formulated as a maximization problem as follows:

$$
\max_u J(u) := \max_u \mathbb{E}[J_{\omega, \theta}(u)]
$$

subject to

$$
\frac{d}{dt}|\psi(\omega, \theta)(t)\rangle = -iH_{\omega, \theta}(t)|\psi(\omega, \theta)(t)\rangle, \quad t \in [0, T], \quad |\psi(\omega, \theta)(0)\rangle = |\psi_0\rangle,
$$

$$
H_{\omega, \theta}(t) = \omega H_0 + \theta \sum_{m=1}^{M} u_m(t)H_m,
$$

$$
\omega \in [1 - \Omega, 1 + \Omega], \quad \theta \in [1 - \Theta, 1 + \Theta],
$$

where $J_{\omega, \theta}(u)$ is a fidelity measure of each member of the ensemble and $\mathbb{E}[J_{\omega, \theta}(u)]$ denotes the average value of $J_{\omega, \theta}$ over the ensemble. The fidelity between the final state $|\psi(\omega, \theta)(T)\rangle$ and the target state $|\psi_{\text{target}}\rangle$ is defined as follows:

$$
F(|\psi(\omega, \theta)(T)\rangle, |\psi_{\text{target}}\rangle) = | \langle \psi(\omega, \theta)(T)|\psi_{\text{target}}\rangle |^2.
$$

The fidelity $F$ is used to evaluate the performance of a designed control in the testing step. However, for convenient calculation of a gradient flow in the training step, we take the performance function $J(u) = F^2$; i.e.,

$$
J_{\omega, \theta}(u) = | \langle \psi(\omega, \theta)(T)|\psi_{\text{target}}\rangle |^2.
$$

Note that $J_{\omega, \theta}$ depends implicitly on the control $u$ through the Schrödinger equation.

B. Sampling-based learning control of inhomogeneous quantum ensembles

Gradient-based methods [4, 38, 40, 41] have been successfully applied to search for optimal solutions to a variety of quantum control problems, including the theoretical and laboratory applications. In this paper, a gradient-based learning method is employed to optimize the controls for inhomogeneous quantum ensembles. We present a systematic methodology for ensemble control design utilizing selected samples (as shown in Fig. 1) from the ensemble. These samples are drawn from the distribution of inhomogeneous parameters to design the control. Then the resultant control is applied to additional ensemble members to test the control performance. As such, the SLC method includes the steps of (i) training and (ii) testing.

1. Training

In the training step, we select $N$ sampled members from the quantum ensemble according to the distribution (e.g., uniform distribution) of the inhomogeneous parameters and then construct a generalized system as
it is necessary to choose a representative set of samples. Using a minimal number of sample members. Therefore, uniform, we may choose some equally spaced samples slice. The time index is \(N\). \(\Omega\) \(N\) \(\Omega\) \(N\) \(\Omega\) \(N\) \(\Omega\)

\[ u(t) = \sum_{n=1}^{N} u_n(t) \]

\[ J_N(u) := \frac{1}{N} \left| \sum_{n=1}^{N} u_n(t) \right|^2 \]

The goal of the training step is to find a control \(u^*\) that maximizes the performance function defined in Eq. (7). The performance function is \(J_N(u)\) with an initial control \(u^0 = \{u_0^0(t)\}\). We apply the gradient flow method \(\text{Algorithm 1}\) to seek an optimal control \(u^* = \{u^*_n(t)\}\). The detailed gradient flow algorithm is provided in the Appendix (Algorithm 1). The time interval \([0, T]\) is divided equally into \(Q\) time slices \(\Delta t\) and we assume that the controls are constant within each time slice. The time index is \(\tau = qT/Q\), where \(Q = T/\Delta t\) and \(q = 1, 2, \ldots, Q\).

The motivation behind SLC is to design the control using a minimal number of sample members. Therefore, it is necessary to choose a representative set of samples. For example, when the distributions of both \(\omega\) and \(\theta\) are uniform, we may choose some equally spaced samples in the \(\omega - \theta\) space. In this case, the intervals of \([1 - \Omega, 1 + \Omega]\) and \([1 - \Theta, 1 + \Theta]\) are divided into \(N_{\Omega1} + 1\) and \(N_{\Theta1} + 1\) subintervals, respectively, where \(N_{\Omega1}\) and \(N_{\Theta1}\) are conveniently chosen positive odd integers. Then the total number of samples is \(N = N_{\Omega1}N_{\Theta1}\), where \(\omega_n\) and \(\theta_n\) are chosen from all combinations of \((\omega_{n1}, \theta_{n1})\) as follows

\[ \omega_n \in \{\omega_{n2} + \Omega, \ldots, (2n_{\Omega} - 1)\Omega\}, \quad n_{\Omega} = 1, 2, \ldots, N_{\Omega} \}

\[ \theta_n \in \{\theta_{n2} + \Theta, \ldots, (2n_{\Theta} - 1)\Theta\}, \quad n_{\Theta} = 1, 2, \ldots, N_{\Theta} \}

\text{Algorithm 1}

2. Testing

For testing, we apply the optimal control \(u^*\) obtained in the training step to additional samples randomly selected from the inhomogeneous quantum ensemble and evaluate the control performance of each sample in terms of the fidelity \(F(|\psi(T)\rangle, |\psi_{\text{target}}\rangle)\) between the final state achieved by each sample \(|\psi(T)\rangle\) and the target state \(|\psi_{\text{target}}\rangle\). If both the average value and the minimum value of the fidelity \(F(|\psi(T)\rangle, |\psi_{\text{target}}\rangle)\) for all the tested samples are satisfactory, we accept the designed control law and end the control design process. Otherwise, we return to the training step and generate another optimized control strategy (e.g., restarting the training step with a new initial control strategy or a new set of samples guided by the performance of the tested members).

III. CONTROL OF TWO-LEVEL INHOMOGENEOUS QUANTUM ENSEMBLES

In this section, we apply SLC to two-level inhomogeneous ensembles. Several groups of numerical experiments are given to evaluate the performance of SLC.

A. Two-level inhomogeneous ensemble

Consider a quantum ensemble consisting of two-level quantum systems (e.g., spins). The Pauli matrices \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) are denoted as follows:

\[ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]

We let the free Hamiltonian be \(H_0 = \frac{1}{2}\sigma_z\) and its two eigenstates are denoted as \(|0\rangle\) and \(|1\rangle\). The control Hamiltonian is \(H_u = \frac{1}{2}v_1(t)\sigma_x + \frac{1}{2}v_2(t)\sigma_y\). Then we have

\[ |\psi(t)\rangle = -iH(t)|\psi(t)\rangle, \]

where \(H(t) = H_0 + H_u(t) = \frac{1}{2}\sigma_z + \frac{1}{2}v_1(t)\sigma_x + \frac{1}{2}v_2(t)\sigma_y\).

For the inhomogeneous ensemble, the Hamiltonian of each member is described as

\[ H_{\omega, \theta}(t) = \omega H_0 + \theta H_u(t). \]

The state of the quantum system can be represented as \(|\psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle\). Denote \(C(t) = (c_0(t), c_1(t))^T\), where \(c_0(t)\) and \(c_1(t)\) are complex amplitudes. We have

\[ i\dot{C}(t) = (H_0 + H_u(t))C(t). \]
To construct a generalized system for the training step, we select $N$ members ($n = 1, 2, \ldots, N$) from the ensemble as follows:

$$
\begin{pmatrix}
    c_{0,n}(t) \\
    c_{1,n}(t)
\end{pmatrix} = \begin{pmatrix}
    0.5\omega_n i & \theta_n f(u) \\
    -\theta_n f^*(u) & -0.5\omega_n i
\end{pmatrix} \begin{pmatrix}
    c_{0,n}(t) \\
    c_{1,n}(t)
\end{pmatrix},
$$

where $f(u) = u_2(t) - 0.5iu_1(t)$, $\omega_n \in [1 - \Omega, 1 + \Omega]$ and $\theta_n \in [1 - \Theta, 1 + \Theta]$ have uniform distributions. The objective is to find a control $u(t) = \{u_m(t), m = 1, 2\}$ to drive all the inhomogeneous members from an initial state $|\psi_0\rangle = |0\rangle$; i.e., $C_0 = (1, 0)^T$, to the target state $|\psi_{\text{target}}\rangle = |1\rangle$; i.e., $C_{\text{target}} = (0, 1)^T$. We construct a generalized system for the training samples using Eq. (6) with the performance function $J_N(u)$ in Eq. (7).

The task is to find the control $u(t)$ to maximize the performance function $J_N(u)$. For a given small threshold $\epsilon > 0$, if $J_N(u) > 1 - \epsilon$, we find a suitable candidate control law for the generalized system. We employ Algorithm 1 to find the optimal control $u^*(t) = \{u^*_m(t), m = 1, 2\}$ for this generalized system. This optimal control is then applied to other randomly selected members to test its performance.

**B. Numerical results**

Several groups of numerical experiments are carried out on an inhomogeneous spin ensemble to demonstrate SLC. The parameter settings are as follows: $\Omega = 0.2$ and $\Theta = 0.2$; the target time is $T = 2$ and the total time interval $[0, T]$ is divided equally into $Q = 200$ time steps, $\Delta t = T/Q = 0.01$; the learning rate is set as $\eta^k = 0.2$; the control strategy is initialized as $u^{k=0}(t) = \{u^0_1(t) = \sin t, u^0_2(t) = \sin t\}$.

**1. Performance with two controls**

To construct a generalized system for the inhomogeneous ensemble with parameter dispersion on both $\omega$ and $\theta$, we choose $N_\omega = 5$ and $N_\theta = 5$ such that $N = N_\omega N_\theta = 25$ samples are employed in the learning phase. Using Eq. (8), we have

$$
\begin{align*}
\omega_n &= 1 - 0.2 + \frac{0.2(\text{fix}(n/5) - 1)}{5}, \\
\theta_n &= 1 - 0.2 + \frac{0.2(\text{mod}(n, 5) - 1)}{5},
\end{align*}
$$

where $n = 1, 2, \ldots, 25$, $\text{fix}(x) = \max\{z \in \mathbb{Z} | z \leq x\}$, $\text{mod}(n, 5) = n - 5z$ ($z \in \mathbb{Z}$ and $\frac{5}{2} - 1 < z \leq \frac{5}{2}$) and $\mathbb{Z}$ is the set of integers. We set $\epsilon = 5 \times 10^{-5}$. The learned optimal control strategy is given as in Fig. 2 and the testing performance in Fig. 3 shows that the fidelities for the state transition lie in the interval of $[0.9985, 1]$ with mean value of 0.9997. For comparison, if we use only one sample ($\omega = 1, \theta = 1$) for training to obtain a control law, the testing performance gives fidelities that lie in $[0.9436, 1]$ with mean value of 0.9808.

These numerical results show that SLC is effective for control design of the two-level inhomogeneous ensemble. The fidelities of the controlled state for the randomly selected members can approach very near to 1 even with $\pm 20\%$ of parameter dispersion with a uniform distribution on all the parameters.

Using the optimal control strategy in Fig. 2, we randomly select several thousand members and present the state transition trajectories of the two-level ensemble on the Bloch sphere. For a two-level system on the Bloch sphere, its state can be represented using a vector $r = (x, y, z)$ where $x = \text{tr}\{|\psi\rangle\langle\psi|\sigma_x\}$, $y = \text{tr}\{|\psi\rangle\langle\psi|\sigma_y\}$, $z = \text{tr}\{|\psi\rangle\langle\psi|\sigma_z\}$. As shown in Fig. 4, although the trajectories of these randomly selected members considerably differ from each other due to the inhomogeneity of the ensemble, they are all successfully driven from the initial state $|\psi_0\rangle = |0\rangle$ (i.e., $r_0 = (0, 0, 1)$) to the same
target state $|ψ_{\text{target}}\rangle = |1\rangle$ (i.e., $r_{\text{target}} = (0, 0, -1)$) with high fidelities indicated above.

2. Performance with $u_1(t) = u_2(t)$

Here we consider only one control, i.e., let $u(t) = u_1(t) = u_2(t)$ with the evolution equation of the ensemble being

$$
\begin{pmatrix}
    \dot{c}_0(t) \\
    \dot{c}_1(t)
\end{pmatrix} =
\begin{pmatrix}
    0.5\omega i & \theta h(u) \\
    -\theta h^*(u) & -0.5\omega i
\end{pmatrix}
\begin{pmatrix}
    c_0(t) \\
    c_1(t)
\end{pmatrix},
$$

where $h(u) = u(t) - 0.5i\dot{u}(t)$. We apply the same SLC design method and parameter settings as in Section III.B.1 except that $\epsilon = 2.0 \times 10^{-2}$. The optimal control strategy is shown in Fig. 5, and Fig. 6 gives the testing performance of 300 randomly selected testing members, whose fidelities lie in $[0.9727, 1]$ with mean value 0.9939. Upon comparison with the case in Section III.B.1, the restricted control has reduced the attainable fidelity.

IV. CONTROL OF THREE-LEVEL INHOMOGENEOUS QUANTUM ENSEMBLES

In this section, we further demonstrate SLC with a Λ-type three-level inhomogeneous ensemble. We conclude this section with a summary of the state transition control fidelities for all the cases in the paper.

A. Control of a Λ-type atomic ensemble

We consider a Λ-type atomic ensemble and demonstrate the SLC design process. For a Λ-type atomic system $^{12}$, $^{13}$, we assume that the initial state is $|ψ(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle + c_3(t)|3\rangle$, and denote $C(t) = (c_1(t), c_2(t), c_3(t))$ where $c_i(t)$’s are complex amplitudes. We have

$$
i\dot{C}(t) = (H_0 + H_u(t))C(t).$$

We take $H_0 = \text{diag}(1.5, 1, 0)$ and choose $H_1$ and $H_2$ in the control Hamiltonian of Eq. [3] as follows $^{12}$:

$$
H_1 = \begin{pmatrix}
    0 & 0 & 0 \\
    0 & 1 & 0 \\
    0 & 0 & 1
\end{pmatrix},
H_2 = \begin{pmatrix}
    0 & 0 & 1 \\
    0 & 0 & 0 \\
    1 & 0 & 0
\end{pmatrix}.
$$

To construct a generalized system for the SLC training step, we choose $N$ samples from the ensemble to form:

$$
\begin{pmatrix}
    \dot{c}_{1,n}(t) \\
    \dot{c}_{2,n}(t) \\
    \dot{c}_{3,n}(t)
\end{pmatrix} =
\begin{pmatrix}
    -1.5\omega_n i & 0 & -i\theta_n u_2(t) \\
    0 & -\omega_n i & -i\theta_n u_1(t) \\
    -i\theta_n u_2(t) & -i\theta_n u_1(t) & 0
\end{pmatrix}
\begin{pmatrix}
    c_{1,n}(t) \\
    c_{2,n}(t) \\
    c_{3,n}(t)
\end{pmatrix},
$$

where $\omega_n \in [1 - \Omega, 1 + \Omega]$ and $\theta_n \in [1 - \Theta, 1 + \Theta]$ have uniform distributions. The objective is to find a control
strategy \( u(t) = \{u_m(t), m = 1, 2\} \) to drive all the inhomogeneous members from \(|\psi_0\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle)\) (i.e., \( C_0 = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}) \)) to \(|\psi_{\text{target}}\rangle = |3\rangle\) (i.e., \( C_{\text{target}} = (0, 0, 1) \)). We aim to maximize the performance function \( J_N(u) \) in Eq. (7) and employ Algorithm 1 to find the optimal control \( u^* (t) = \{u_m^*(t), m = 1, 2\} \) for this generalized system. Then the optimal control strategy is applied to other randomly selected members to test its performance.

**B. Numerical example**

We use the parameter settings as follows: the control strategy is initialized with \( u^{k=0}(t) = \{u_m^0(t) = \sin t, m = 1, 2\}; \epsilon = 10^{-4}; \) the other parameter settings are the same as those of the numerical experiments for the spin ensemble in Section III. To construct a generalized system for the training step, we have the training samples selected as follows

\[
\begin{align*}
\omega_n &= 1 - 0.2 + \frac{0.2(2\text{fix}(n/5) - 1)}{5}, \\
\theta_n &= 1 - 0.2 + \frac{0.2(2\text{mod}(n, 5) - 1)}{5},
\end{align*}
\]

(19)

where \( n = 1, 2, \ldots, 25 \). The learned optimal control strategy is given in Fig. 7 and the testing results are shown in Fig. 8, which shows the fidelities for all the 300 testing members lie in the interval of \([1 - 10^{-6}, 1]\). For the case with parameter dispersion only in \( \omega \), the fidelities lie in the interval of \([0.9987, 1]\) with the mean value 0.9994. If only \( u_1(t) = u_2(t) \) is allowed, the control performance is not as good as that with two controls \( u_1(t) \) and \( u_2(t) \) since we have fewer adjustable degrees of freedom. All these numerical results further demonstrate previous theoretical predictions that ensemble control should be feasible [31]-[33].

**V. CONCLUSIONS**

In this paper, we presented a systematic methodology for control design of inhomogeneous quantum ensembles. The proposed SLC method includes the steps of (i) training and (ii) testing. In the training step, the control is learned for a generalized system constructed from samples using a gradient flow based learning and optimiza-
tion algorithm. In the process of testing, the control obtained in the first step is evaluated for more randomly selected members. One approach would be to first learn off-line a control field using the SLC method, and then generate and apply the control field to an inhomogeneous quantum ensemble in the laboratory.

Appendix: Gradient flow methods for quantum ensemble control

To get an optimal control strategy \( u^* = \{ u_m^n(t), t \in [0, T], m = 1, 2, \ldots, M \} \) for the generalized system \([6]\), one technique is to follow the gradient of \( J_N(u) \) as an ascent direction. For ease of notation, we present the method for \( M = 1 \). We introduce a time-like variable \( s \) to characterize different control strategies \( u(s) \). Then a gradient flow in the control space is defined as

\[
\frac{du(s)}{ds} = \nabla J_N(u(s)),
\]

(20)

where \( \nabla J_N(u) \) denotes the gradient of \( J_N \) with respect to the control \( u \). If \( u(s) \) is the solution of \([21]\) starting from an arbitrary initial condition \( u(0) \), then the value of \( J_N \) will increase along \( u(s) \); i.e., \( \frac{d}{ds} J_N(u(s)) \geq 0 \). Starting from a trial guess \( u^0 \), we solve the following initial value problem

\[
\begin{cases}
\frac{du(s)}{ds} = \nabla J_N(u(s)), \\
u(0) = u^0
\end{cases}
\]

(21)

in order to find a control strategy which maximizes \( J_N \). This initial value problem can then be solved numerically by using a forward Euler method (or, if necessary, a high order integration method) over the \( s \)-domain; i.e.,

\[
u(s + \Delta s, t) = u(s, t) + \Delta s \nabla J_N(u(s)).
\]

(22)

In practical applications, in term of a discrete update iteration index \( k \), equation \([22]\) can be rewritten as

\[
u^{k+1}(t) = \nu^k(t) + \eta^k \nabla J_N(\nu^k),
\]

(23)

where \( \eta^k \) is the updating stepsize (learning rate) for the \( k \)th iteration. By Eq. \([7]\), we also obtain that

\[
\nabla J_N(u) = \frac{1}{N} \sum_{n=1}^{N} \nabla J_{\omega_n, \theta_n}(u),
\]

(24)

In addition, we have

\[
\nabla J_{\omega_n, \theta_n}(u) = 2 \Im \langle \langle \psi_{\omega_n, \theta_n}(T) \vert \psi_{\text{target}} \rangle \langle \psi_{\text{target}} \vert A(t) \vert \psi_u \rangle \rangle
\]

(25)

where \( A(t) = U_{\omega_n, \theta_n}(T) U_{\omega_n, \theta_n}^\dagger \theta_n H U_{\omega_n, \theta_n}(t) \), \( \Im \langle \cdot \rangle \) denotes the imaginary part of a complex number, and the propagator \( U_{\omega_n, \theta_n}(t) \) satisfies

\[
\frac{d}{dt} U_{\omega_n, \theta_n}(t) = -i H U_{\omega_n, \theta_n}(t), \quad U(0) = \text{Id}.
\]

The gradient flow method can be generalized to the case with \( M > 1 \) as shown in Algorithm 1.

**Algorithm 1** Gradient flow based iterative learning

1: Set the iteration index \( k = 0 \)
2: Choose a set of arbitrary controls \( u^{k=0} = \{u^0_m(t), \ m = 1, 2, \ldots, M\}, \ t \in [0, T] \)
3: repeat (for each iterative process)
4: \hspace{1cm} repeat (for each training sample member \( n = 1, 2, \ldots, N \))
5: \hspace{2cm} Compute the propagator \( U^k_n(t) \) with the control strategy \( u^k(t) \)
6: \hspace{1cm} until \( n = N \)
7: \hspace{1cm} repeat (for each control \( u_m \ (m = 1, 2, \ldots, M) \) of the vector \( u \))
8: \hspace{2cm} \( \delta^k_m(t) = 2 \Im \langle \langle \psi_{\omega_n, \theta_n}(T) \vert \psi_{\text{target}} \rangle \langle \psi_{\text{target}} \vert A_m(t) \vert \psi_u \rangle \rangle \)
9: \hspace{2cm} where \( A_m(t) = U_{\omega_n, \theta_n}(T) U_{\omega_n, \theta_n}^\dagger \theta_n H U_{\omega_n, \theta_n}(t) \)
10: \hspace{2cm} \( u^{k+1}_m(t) = u^k_m(t) + \eta^k \delta^k_m(t) \)
11: \until \( m = M \)
12: \until \ the learning process ends
13: The optimal control strategy \( u = \{u^*_m\} = \{u^k_m\}, \ m = 1, 2, \ldots, M \)

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