2014 International Joint Conference on Neural Networks (IJCNN)
July 6-11, 2014, Beijing, China

Sampling-based learning control for quantum discrimination and ensemble classification

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***Abstract*—Quantum ensemble classification has significant applications in discrimination of atoms (or molecules), separation of isotopic molecules and quantum information extraction. In this paper, we recast quantum ensemble classification as a supervised quantum learning problem. A systematic classification methodology is presented by using a sampling-based learning control (SLC) approach for quantum discrimination. The classification task is accomplished via simultaneously steering members belonging to different classes to their corresponding target states (e.g., mutually orthogonal states). Numerical results demonstrate the effectiveness of the proposed approach for the discrimination of two quantum systems and the binary classification of two-level quantum ensembles.**

***Keywords*—Ensemble classification, quantum discrimination, inhomogeneous ensembles, sampling-based learning control.**

I. Introduction

Optimal discrimination [1], [2] and classification [3] of quantum states or quantum systems is a central topic in quantum information technology [4]-[7]. In existing research, discrimination of two similar quantum systems (e.g., similar molecules) has been extensively investigated [8]-[15]. Many practical quantum systems exist in the form of quantum ensembles. A quantum ensemble consists of a large number of (e.g., 10^{23}) single quantum systems (members). Quantum ensembles have wide applications in emerging quantum technology including quantum computation [16], long-distance quantum communication [17], and magnetic resonance imaging [18]. In practical applications, the members of a quantum ensemble could show variations in the parameters that characterize the system dynamics [19], [20]. Such an ensemble is called an inhomogeneous quantum ensemble [21]. The classification of inhomogeneous quantum ensembles is a significant issue and has great potential applications in the discrimination of atoms (or molecules), the separation of isotopic molecules and quantum information extraction.

However, quantum mechanics forbids deterministic discrimination among nonorthogonal states [1]. A useful idea is to first drive the members of a quantum ensemble from an initial state to different orthogonal states corresponding to different classes (e.g., eigenstates) before classifying them. Usually, it is impractical to employ different control inputs for individual members of a quantum ensemble in physical experiments. Hence, it is important to develop new approaches for designing external control fields that can simultaneously steer the ensemble of inhomogeneous systems from an initial state to different target states when variations exist in their internal parameters. Some quantum control techniques such as the multidimensional pseudospectral method [18], [22] and the sampling-based learning control approach [21] may provide inspiration for the solution to this problem.

In this paper, we recast the quantum ensemble classification task as a supervised quantum learning problem and present a systematic classification methodology by using a sampling-based learning control (SLC) method [21], [23] in quantum discrimination. In this method, we first learn an optimal control strategy to steer the members in a quantum ensemble belonging to different classes into their corresponding target states, and then employ a physical read-out process (e.g., Stern-Gerlach experiment [4]) to classify these classes.

This paper is organized as follows. Section II formulates the learning problem for quantum ensemble classification. A control design method is presented in Section III for quantum discrimination of similar quantum systems. In Section IV an SLC method is proposed for the binary classification of quantum ensembles and numerical results are demonstrated for a spin ensemble. Conclusions are presented in Section V.

II. Problem formulation

We focus on finite-dimensional closed quantum systems with the following dynamics (setting the constant $\hbar = 1$):

$$\begin{cases} \frac{d}{dt}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle \\ t \in [0,T],\ |\psi(0)\rangle = |\psi_0\rangle \end{cases} \tag{1}$$

where $|\psi(t)\rangle$ (quantum state) is a unit complex vector on the underlying Hilbert space, $H(t)$ is the system Hamiltonian and $i = \sqrt{-1}$. The dynamics of the system is governed by a time-dependent Hamiltonian of the form

$$H(t) = H_0 + H_c(t) = H_0 + \sum_{m=1}^{M} u_m(t) H_m, \tag{2}$$

where H_0 is the free Hamiltonian of the system and $H_c(t) = \sum_{m=1}^{M} u_m(t) H_m$ is the time-dependent control Hamiltonian that represents the interaction of the system with the external fields $u_m(t)$. H_m are Hermitian operators through which the controls couple to the system. The solution of (1) is given by $|\psi(t)\rangle = U(t)|\psi_0\rangle$, where the propagator $U(t)$ satisfies the following equation ($U(0) = I$ and I is an identity matrix)

$$\frac{d}{dt}U(t) = -iH(t)U(t). \tag{3}$$

In this paper, we consider the classification problem for a quantum ensemble of similar members with different Hamiltonians, which is referred to as *quantum ensemble classification* (QEC). Suppose that for an inhomogeneous quantum ensemble, we are given an unknown member belonging to a certain class, how well can we predict the class that the unknown member belongs to? We have to drive the members from different classes to appropriate orthogonal states (e.g., eigenstates) before we can discriminate them with high accuracy. The sampling-based learning control approach presented for the control of inhomogeneous quantum ensembles can be combined with supervised learning for QEC. We denote a training set as $D_N = \{(H^1(t), y_1), (H^2(t), y_2), \dots, (H^N(t), y_N)\}$ which consists of N quantum systems (each of them labeled with an associated class). $H^n(t)$ ($n = 1, 2, \dots, N$) describes the nth quantum system in the training set and y_n is the associated class that this quantum system belongs to.

For simplicity, we consider an inhomogeneous ensemble consisting of two classes of members (i.e., classes A and B) and propose an SLC approach for this binary quantum ensemble classification problem using a spin-$\frac{1}{2}$ quantum ensemble example. Assume that the Hamiltonian of each member has the following form

$$\begin{cases} H^A_{\varepsilon_0,\varepsilon_u}(t) = g^A_0(\varepsilon_0)H_0 + g^A_u(\varepsilon_u)\sum_{m=1}^{M} u_m(t)H_m \\ H^B_{\varepsilon_0,\varepsilon_u}(t) = g^B_0(\varepsilon_0)H_0 + g^B_u(\varepsilon_u)\sum_{m=1}^{M} u_m(t)H_m. \end{cases} \tag{4}$$

$g^A_0(\cdot)$ and $g^A_u(\cdot)$ are known functions, while the inhomogeneity parameters ε_0 and ε_u in the Hamiltonian $H^A_{\varepsilon_0,\varepsilon_u}(t)$ for class A are characterized by the distribution functions $d^A_0(\varepsilon_0)$ and $d^A_u(\varepsilon_u)$, respectively. We assume that the parameters ε_0 and ε_u are time independent. A similar expression to (4) is defined for the Hamiltonian $H^B_{\varepsilon_0,\varepsilon_u}(t)$ of class B.

For a binary quantum ensemble classification task, the objective is to design a control strategy $u(t) = \{u_m(t), m = 1, 2, \dots, M\}$ to simultaneously stabilize the members in class A (with different ε_0 and ε_u) from an initial state $|\psi_0\rangle$ to the same target state $|\psi_{\text{targetA}}\rangle$, and at the same time to stabilize the members in class B (with different ε_0 and ε_u) from $|\psi_0\rangle$ to another target state $|\psi_{\text{targetB}}\rangle$. A binary quantum ensemble classification (binary QEC) task is to construct a binary quantum classifier to maximize the classification accuracy. The key task of a binary QEC is to learn an optimal control strategy in the training step for the binary quantum classifier. The training performance is described by a *performance function* $J(u)$ for each learned control strategy $u = \{u_m(t), m = 1, 2, \dots, M\}$. The binary QEC problem can then be formulated as a maximization problem as follows:

$$\begin{aligned} &\max_u J(u) := \max_u \{w_A \mathbb{E}[J^A_{\varepsilon_0,\varepsilon_u}(u)] + w_B \mathbb{E}[J^B_{\varepsilon_0,\varepsilon_u}(u)]\} \\ \text{s.t.}\quad & t \in [0,T] \quad |\psi^A_{\varepsilon_0,\varepsilon_u}(0)\rangle = |\psi^B_{\varepsilon_0,\varepsilon_u}(0)\rangle = |\psi_0\rangle \\ & \begin{cases} \frac{d}{dt}|\psi^A_{\varepsilon_0,\varepsilon_u}(t)\rangle = -iH^A_{\varepsilon_0,\varepsilon_u}(t)|\psi^A_{\varepsilon_0,\varepsilon_u}(t)\rangle \\ H^A_{\varepsilon_0,\varepsilon_u}(t) = g^A_0(\varepsilon_0)H_0 + g^A_u(\varepsilon_u)\sum_{m=1}^{M} u_m(t)H_m \\ J^A_{\varepsilon_0,\varepsilon_u}(u) := |\langle\psi^A_{\varepsilon_0,\varepsilon_u}(T)|\psi_{\text{targetA}}\rangle|^2 \end{cases} \\ & \begin{cases} \frac{d}{dt}|\psi^B_{\varepsilon_0,\varepsilon_u}(t)\rangle = -iH^B_{\varepsilon_0,\varepsilon_u}(t)|\psi^B_{\varepsilon_0,\varepsilon_u}(t)\rangle \\ H^B_{\varepsilon_0,\varepsilon_u}(t) = g^B_0(\varepsilon_0)H_0 + g^B_u(\varepsilon_u)\sum_{m=1}^{M} u_m(t)H_m \\ J^B_{\varepsilon_0,\varepsilon_u}(u) := |\langle\psi^B_{\varepsilon_0,\varepsilon_u}(T)|\psi_{\text{targetB}}\rangle|^2 \end{cases} \end{aligned} \tag{5}$$

where $w_A, w_B \in [0,1]$ are the weights assigned to classes A and B, respectively, satisfying $w_A + w_B = 1$. $J^A_{\varepsilon_0,\varepsilon_u}(u)$ is a measure of classification accuracy for each member in class A regarding the target state $|\psi_{\text{targetA}}\rangle$ and $\mathbb{E}[J^A_{\varepsilon_0,\varepsilon_u}(u)]$ denotes the average value of $J^A_{\varepsilon_0,\varepsilon_u}(u)$ over class A. A similar expression holds for class B. The performance $J(u)$ represents the weighted accuracy of classification.

III. Discrimination of two similar quantum systems

Optimal dynamic discrimination between two similar quantum systems has been investigated using different techniques [2], [8]. The quantum discrimination problem can be taken as a special case of the binary QEC problem with the number of members in an ensemble $N_e = 2$. In this section, we develop a gradient-based learning control method for quantum discrimination of two similar quantum systems.

A. Learning control design for quantum discrimination

Suppose two similar quantum systems to be discriminated a and b have the following Hamiltonians:

$$\begin{cases} H^a_{\varepsilon^a_0,\varepsilon^a_u}(t) = g_0(\varepsilon^a_0)H_0 + g_u(\varepsilon^a_u)\sum_{m=1}^{M} u_m(t)H_m \\ H^b_{\varepsilon^b_0,\varepsilon^b_u}(t) = g_0(\varepsilon^b_0)H_0 + g_u(\varepsilon^b_u)\sum_{m=1}^{M} u_m(t)H_m \end{cases} \tag{6}$$

where ε^a_0, ε^a_u, ε^b_0 and ε^b_u are predefined constants for functions $g_0(\cdot)$ and $g_u(\cdot)$. a and b are prepared in the same initial state

$|\psi_0\rangle$. The objective is to find an optimal control strategy $u(t)$ ($t \in [0,T]$) to drive the state of system a to the target state $|\psi_{\text{targetA}}\rangle$ and the state of system b to the target state $|\psi_{\text{targetB}}\rangle$ at the same time. Usually, we let $\langle\psi_{\text{targetA}}|\psi_{\text{targetB}}\rangle = 0$ so that we can completely discriminate system a from system b. The control performance $J(u)$ is redefined for the discrimination problem as

$$J(u) := w_a J^a_{\varepsilon_0^a,\varepsilon_u^a}(u) + w_b J^b_{\varepsilon_0^b,\varepsilon_u^b}(u) \tag{7}$$

where $w_a, w_b \in [0,1]$ are the weights assigned to the associated systems, respectively, and

$$\begin{aligned} J^a_{\varepsilon_0^a,\varepsilon_u^a}(u) &:= |\langle\psi^a_{\varepsilon_0^a,\varepsilon_u^a}(T)|\psi_{\text{targetA}}\rangle|^2, \\ J^b_{\varepsilon_0^b,\varepsilon_u^b}(u) &:= |\langle\psi^b_{\varepsilon_0^b,\varepsilon_u^b}(T)|\psi_{\text{targetB}}\rangle|^2. \end{aligned} \tag{8}$$

Here we set $w_a = w_b = 0.5$ for the discrimination problem.

In order to find an optimal control strategy $u^* = \{u_m^*(t), (t \in [0,T]), m = 1,2,\ldots,M\}$ for the discrimination problem, it is a good choice to follow the direction of the gradient of $J(u)$ 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 $u^{(s)}(t)$. Then a gradient flow in the control space can be defined as

$$\frac{du^{(s)}}{ds} = \nabla J(u^{(s)}), \tag{9}$$

where $\nabla J(u)$ denotes the gradient of $J(u)$ with respect to the control u. Starting from an initial guess u^0, we solve the following initial value problem

$$\begin{cases} \dfrac{du^{(s)}}{ds} = \nabla J(u^{(s)}) = w_a \nabla J^a_{\varepsilon_0^a,\varepsilon_u^a}(u^{(s)}) + w_b \nabla J^b_{\varepsilon_0^b,\varepsilon_u^b}(u^{(s)}) \\ u^{(0)} = u^0 \end{cases} \tag{10}$$

in order to find a control strategy which maximizes $J(u)$. This initial value problem can then be solved numerically by a forward Euler method over the s-domain, i.e.,

$$u(s + \triangle s, t) = u(s,t) + \triangle s \nabla J(u^{(s)}). \tag{11}$$

As for practical applications, we present its iterative approximation version to find the optimal control $u^*(t)$, where we use k as an index of iterations instead of the variable s and denote the control at iteration step k as $u^k(t)$. Equation (11) can be rewritten as

$$u^{k+1}(t) = u^k(t) + \eta_k \nabla J(u^k), \tag{12}$$

where η_k is the updating step (learning rate) for the kth iteration and

$$\nabla J(u^k) = w_a \nabla J^a_{\varepsilon_0^a,\varepsilon_u^a}(u^k) + w_b \nabla J^b_{\varepsilon_0^b,\varepsilon_u^b}(u^k). \tag{13}$$

In addition, we have the gradient of $J^a_{\varepsilon_0^a,\varepsilon_u^a}(u^k)$ with respect to the control u as follows (for more details, see, e.g., [21])

$$\nabla J^a_{\varepsilon_0^a,\varepsilon_u^a}(u^k) = 2\Im\left(\langle\psi^a_{\varepsilon_0^a,\varepsilon_u^a}(T)|\psi_{\text{targetA}}\rangle\langle\psi_{\text{targetA}}|G_1^a(t)|\psi_0\rangle\right), \tag{14}$$

where $\Im(\cdot)$ denotes the imaginary part of a complex number, $G_1^a(t) = U_{\varepsilon_0^a,\varepsilon_u^a}(T)U^\dagger_{\varepsilon_0^a,\varepsilon_u^a}(t) g_u(\varepsilon_u^a) H_1 U_{\varepsilon_0^a,\varepsilon_u^a}(t)$, and the propagator $U_{\varepsilon_0^a,\varepsilon_u^a}(t)$ satisfies

$$\frac{d}{dt}U_{\varepsilon_0^a,\varepsilon_u^a}(t) = -iH^a_{\varepsilon_0^a,\varepsilon_u^a}(t)U_{\varepsilon_0^a,\varepsilon_u^a}(t), \quad U(0) = I.$$

A similar expression can also be derived for $\nabla J^b_{\varepsilon_0^b,\varepsilon_u^b}(u^k)$. When we generalize the gradient flow method to the case with $M > 1$, for each control $u_m(t)$ ($m = 1,2,\ldots,M$) of the control strategy $u(t)$, we have

$$\begin{aligned} \nabla J(u_m^k) = & 2w_a \Im\left(\langle\psi^a_{\varepsilon_0^a,\varepsilon_u^a}(T)|\psi_{\text{targetA}}\rangle\langle\psi_{\text{targetA}}|G_m^a(t)|\psi_0\rangle\right) \\ & + 2w_b \Im\left(\langle\psi^b_{\varepsilon_0^b,\varepsilon_u^b}(T)|\psi_{\text{targetB}}\rangle\langle\psi_{\text{targetB}}|G_m^b(t)|\psi_0\rangle\right) \end{aligned} \tag{15}$$

where

$$G_m^a(t) = U_{\varepsilon_0^a,\varepsilon_u^a}(T)U^\dagger_{\varepsilon_0^a,\varepsilon_u^a}(t) g_u(\varepsilon_u^a) H_m U_{\varepsilon_0^a,\varepsilon_u^a}(t),$$

$$G_m^b(t) = U_{\varepsilon_0^b,\varepsilon_u^b}(T)U^\dagger_{\varepsilon_0^b,\varepsilon_u^b}(t) g_u(\varepsilon_u^b) H_m U_{\varepsilon_0^b,\varepsilon_u^b}(t).$$

A gradient flow based iterative learning algorithm for the discrimination of quantum systems is shown in *Algorithm 1*.

Algorithm 1. Gradient flow based iterative learning for quantum discrimination

Set the index of iterations $k = 0$
Choose a set of arbitrary controls $u^{k=0}(t) = \{u_m^0(t),\ m = 1,2,\ldots,M\}, t \in [0,T]$
repeat (for each iterative process)
  Compute the propagator $U^k_{\varepsilon_0^a,\varepsilon_u^a}(t)$ and $U^k_{\varepsilon_0^b,\varepsilon_u^b}(t)$ for systems a and b, respectively, with the control strategy $u^k(t)$
  repeat (for each control $u_m(t)$ ($m = 1,2,\ldots,M$) of the control vector $u^k(t)$)
    $\delta_m^k(t) := \nabla J(u_m^k)$ and compute $\nabla J(u_m^k)$ using equation (15)
    $u_m^{k+1}(t) = u_m^k(t) + \eta_k \delta_m^k(t)$
  until $m = M$
  $k = k+1$
until the learning process ends
The optimal control strategy $u^*(t) = \{u_m^*(t)\} = \{u_m^k(t)\},\ m = 1,2,\ldots,M$

Remark 1: In the practical implementation, we usually divide the time duration $[0,T]$ equally into a number of time slices $\triangle t$ and assume that the controls are constant within each time slice. Instead of $t \in [0,T]$, the time index is $t_q = qT/Q$, where $Q = T/\triangle t$ and $q = 1,2,\ldots,Q$.

B. Numerical examples

To demonstrate this learning control method for discrimination of two similar quantum systems, we consider two-level (spin-$\frac{1}{2}$) systems. We denote the Pauli matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ [4]. For a two-level quantum system, we may assume the free Hamiltonian $H_0 = \frac{1}{2}\sigma_z$. Its two eigenstates are denoted as $|0\rangle$ (e.g., spin up) and $|1\rangle$ (e.g., spin down). To control a two-level quantum system, we use the control Hamiltonian of $H_u = \frac{1}{2}u_1(t)\sigma_x + \frac{1}{2}u_2(t)\sigma_y$. Hence,

$$H(t) = H_0 + H_u(t) = \frac{1}{2}\sigma_z + \frac{1}{2}u_1(t)\sigma_x + \frac{1}{2}u_2(t)\sigma_y. \tag{16}$$

For two similar spin-$\frac{1}{2}$ systems, the Hamiltonian of each system can be described as

$$\begin{aligned} H_{\varepsilon_0,\varepsilon_u}(t) &= g_0(\varepsilon_0)H_0 + g_u(\varepsilon_u)H_u(t) \\ &= \frac{1}{2}g_0(\varepsilon_0)\sigma_z + \frac{1}{2}g_u(\varepsilon_u)(u_1(t)\sigma_x + u_2(t)\sigma_y). \end{aligned} \tag{17}$$

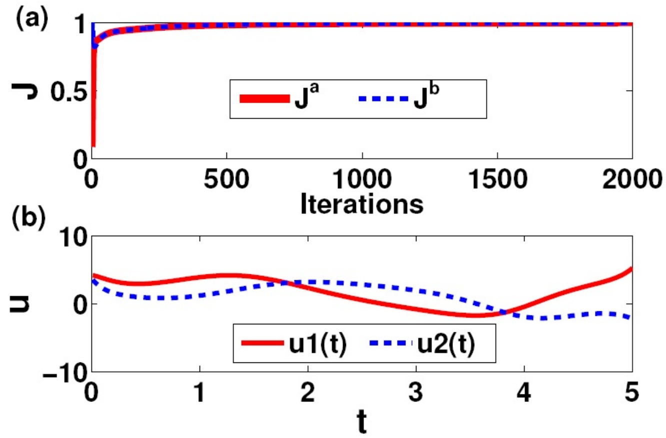

Fig. 1. Learning performance of discrimination between system a ($(\varepsilon_0^a, \varepsilon_u^a) = (0.9, 0.9)$) and system b ($(\varepsilon_0^b, \varepsilon_u^b) = (1.1, 1.1)$). (a) Evolution of performance functions $J^a(u)$ and $J^b(u)$; (b) The learned optimal control strategy $u(t)$.

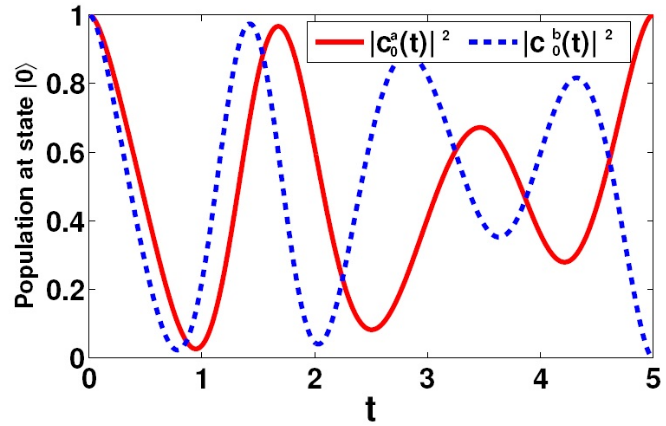

Fig. 2. Evolution of the states of system a ($(\varepsilon_0^a, \varepsilon_u^a) = (0.9, 0.9)$) and system b ($(\varepsilon_0^b, \varepsilon_u^b) = (1.1, 1.1)$) regarding their populations ($|c_0^a(t)|^2$ and $|c_0^b(t)|^2$) at the state $|0\rangle$, respectively.

We assume $g_0(\varepsilon_0) = \varepsilon_0$ and $g_u(\varepsilon_u) = \varepsilon_u$. The state of the two quantum systems can be represented in the eigen-basis of H_0 by $|\psi(t)\rangle = c_0(t)|0\rangle + c_1(t)|1\rangle$. Denote $C(t) = (c_0(t), c_1(t))^T$, where $c_0(t)$ and $c_1(t)$ are complex numbers, and x^T represents the transpose of x. We have

$$\begin{pmatrix} \dot{c}_0(t) \\ \dot{c}_1(t) \end{pmatrix} = \begin{pmatrix} 0.5\varepsilon_0 i & \varepsilon_u f(u) \\ -\varepsilon_u f^*(u) & -0.5\varepsilon_0 i \end{pmatrix} \begin{pmatrix} c_0(t) \\ c_1(t) \end{pmatrix}, \quad (18)$$

where $f(u) = u_2(t) - 0.5iu_1(t)$, $(\varepsilon_0, \varepsilon_u) = (\varepsilon_0^a, \varepsilon_u^a)$ for system a and $(\varepsilon_0, \varepsilon_u) = (\varepsilon_0^b, \varepsilon_u^b)$ for system b.

Define the performance function as

$$\begin{aligned} J(u) &= \frac{1}{2}J^a(u) + \frac{1}{2}J^b(u) \\ &= \frac{1}{2}|\langle C_a(T)|C_{\text{targetA}}\rangle|^2 + \frac{1}{2}|\langle C_b(T)|C_{\text{targetB}}\rangle|^2. \end{aligned} \quad (19)$$

The task is to find a control $u(t)$ to maximize the performance function in (19). For a given small threshold $\varepsilon > 0$, if $|J(u^{k+1}) - J(u^k)| < \varepsilon$ for uninterrupted n_e steps, we may think we find a suitable control law for the problem. In this paper, we set $\varepsilon = 10^{-4}$ and $n_e = 100$ in all numerical experiments.

Now we employ *Algorithm 1* to find the optimal control strategy $u^*(t) = \{u_m^*(t), m = 1, 2\}$ and then apply the optimal control strategy for discriminating system a from system b. The parameter settings are listed as follows: the initial state $C_0 = (1, 0)^T$, i.e., $|\psi_0\rangle = |0\rangle$, and the target state for system a $C_{\text{targetA}} = (1, 0)^T$, i.e., $|\psi_{\text{targetA}}\rangle = |0\rangle$; the target state for system b $C_{\text{targetB}} = (0, 1)^T$, i.e., $|\psi_{\text{targetB}}\rangle = |1\rangle$; The ending time $T = 5$ (in atomic units) and the total time duration $[0, T]$ is equally discretized into $Q = 500$ time slices with each time slice $\Delta t = (t_q - t_{q-1})|_{q=1,2,\ldots,Q} = T/Q = 0.01$; the learning rate $\eta_k = 0.2$; the control strategy is initialized as $u^{k=0}(t) = \{u_1^0(t) = \sin t, u_2^0(t) = \sin t\}$.

In the example, two similar systems a and b are characterized with parameters $(\varepsilon_0^a, \varepsilon_u^a) = (0.9, 0.9)$ and $(\varepsilon_0^b, \varepsilon_u^b) = (1.1, 1.1)$, respectively. The numerical results are shown in Fig. 1 and Fig. 2. As shown in Fig. 1(a), the learning process converges very quickly and the performance function $J(u)$ converges to 0.999 after about 2000 steps of iterative learning with an optimized control strategy $u(t) = \{u_1(t), u_2(t)\}$ in Fig. 1(b). Then we apply the learned optimal control strategy to systems a and b. The evolution of their states can be clearly demonstrated regarding their populations at the state $|0\rangle$ as shown in Fig. 2. At time $t = T = 5$, $|c_0^a(T)|^2 = 1.0000$ and $|c_0^b(T)|^2 = 0.0000$, which indicates that, after the coherent control step, we can discriminate system a from system b using a projective measurement and the success probability is almost 100%.

IV. Quantum Ensemble Classification via SLC

Binary classification is to classify the members of a given set of objects into two classes on the basis of whether they have certain properties or not. For a binary QEC problem, we have to learn from a training set and find out an optimal control strategy for all the members in the quantum ensemble. In this section, we combine a sampling-based learning control (SLC) approach into the quantum discrimination method introduced above to solve the QEC problem (i.e., the maximization problem formulated as Equation (5)).

A. SLC for quantum ensemble classification

In the quantum domain, it is difficult to obtain a specific description for a single system in a quantum ensemble, while we can characterize an ensemble of similar systems with a distribution of parameters (e.g., Gaussian distribution, Boltzmann distribution and uniform distribution). According to the distribution of parameters for a quantum ensemble, we can choose sample members to construct the training set for the learning control design. This approach is referred to as sampling-based learning control (SLC), which originated in [21], [23] as a general framework for optimal control design of inhomogeneous quantum ensembles and robust control design of quantum systems with uncertainties.

In the SLC approach, a generalized system is constructed by sampling members from the inhomogeneous ensemble. In this paper, we adopt the key idea from SLC and solve the supervised quantum learning problem of QEC via constructing a generalized system using the training set.

Suppose we have obtained a training set $D_N = \{(H^n(t), y_n)\}$ $(n = 1,2,\dots,N)$ for the binary QEC problem, where $y_n \in \{A,B\}$ and $H^n(t)$ is the time-dependent Hamiltonian that describes the nth member of the quantum ensemble. Now we split D_N into two subsets according to the value of y_n and rewrite the training set as follows

$$\begin{aligned}
&D_N = D_{N_A} \cup D_{N_B},\ N = N_A + N_B,\\
&D_{N_A} = \{(H^A_{\varepsilon_0^{n_A},\varepsilon_u^{n_A}}(t), y_{n_A} = A)\},\ n_A = 1,2,\dots,N_A,\\
&D_{N_B} = \{(H^B_{\varepsilon_0^{n_B},\varepsilon_u^{n_B}}(t), y_{n_B} = B)\},\ n_B = N_A+1, N_A+2,\dots,N,
\end{aligned} \tag{20}$$

where $H^A_{\varepsilon_0^{n_A},\varepsilon_u^{n_A}}(t) = g_0^A(\varepsilon_0^{n_A})H_0 + g_u^A(\varepsilon_u^{n_A})\sum_{m=1}^M u_m(t)H_m$ and $H^B_{\varepsilon_0^{n_B},\varepsilon_u^{n_B}}(t) = g_0^B(\varepsilon_0^{n_B})H_0 + g_u^B(\varepsilon_u^{n_B})\sum_{m=1}^M u_m(t)H_m$.

Using the training set (20), we can construct a generalized system as follows

$$\frac{d}{dt}\begin{pmatrix} |\psi^A_{\varepsilon_0^1,\varepsilon_u^1}(t)\rangle \\ \vdots \\ |\psi^A_{\varepsilon_0^{N_A},\varepsilon_u^{N_A}}(t)\rangle \\ |\psi^B_{\varepsilon_0^{N_A+1},\varepsilon_u^{N_A+1}}(t)\rangle \\ \vdots \\ |\psi^B_{\varepsilon_0^N,\varepsilon_u^N}(t)\rangle \end{pmatrix} = -i\begin{pmatrix} H^A_{\varepsilon_0^1,\varepsilon_u^1}(t)|\psi^A_{\varepsilon_0^1,\varepsilon_u^1}(t)\rangle \\ \vdots \\ H^A_{\varepsilon_0^{N_A},\varepsilon_u^{N_A}}(t)|\psi^A_{\varepsilon_0^{N_A},\varepsilon_u^{N_A}}(t)\rangle \\ H^B_{\varepsilon_0^{N_A+1},\varepsilon_u^{N_A+1}}(t)|\psi^B_{\varepsilon_0^{N_A+1},\varepsilon_u^{N_A+1}}(t)\rangle \\ \vdots \\ H^B_{\varepsilon_0^N,\varepsilon_u^N}(t)|\psi^B_{\varepsilon_0^N,\varepsilon_u^N}(t)\rangle \end{pmatrix}. \tag{21}$$

The performance function for this generalized system is defined by

$$J_N(u) := w_A J^A + w_B J^B, \tag{22}$$

where

$$\begin{aligned}
J^A &= \frac{1}{N_A}\sum_{n_A=1}^{N_A} J^A_{\varepsilon_0^{n_A},\varepsilon_u^{n_A}}(u) = \frac{1}{N_A}\sum_{n_A=1}^{N_A} |\langle\psi^A_{\varepsilon_0^{n_A},\varepsilon_u^{n_A}}(T)|\psi_{\text{targetA}}\rangle|^2,\\
J^B &= \frac{1}{N_B}\sum_{n_B=N_A+1}^{N} J^B_{\varepsilon_0^{n_B},\varepsilon_u^{n_B}}(u) = \frac{1}{N_B}\sum_{n_B=N_A+1}^{N} |\langle\psi^B_{\varepsilon_0^{n_B},\varepsilon_u^{n_B}}(T)|\psi_{\text{targetB}}\rangle|^2.
\end{aligned} \tag{23}$$

Then we design the SLC algorithm (*Algorithm 2*) for binary QEC using the gradient flow method to approximate an optimal control strategy $u^* = \{u_m^*(t)\}$.

B. Numerical examples

We consider two-level quantum systems. For two similar classes of members in an inhomogeneous quantum ensemble, the Hamiltonians can be described as

$$\begin{aligned}
H^A_{\varepsilon_0,\varepsilon_u}(t) &= \frac{1}{2}g_0^A(\varepsilon_0)\sigma_z + \frac{1}{2}g_u^A(\varepsilon_u)(u_1(t)\sigma_x + u_2(t)\sigma_y),\\
H^B_{\varepsilon_0,\varepsilon_u}(t) &= \frac{1}{2}g_0^B(\varepsilon_0)\sigma_z + \frac{1}{2}g_u^B(\varepsilon_u)(u_1(t)\sigma_x + u_2(t)\sigma_y).
\end{aligned} \tag{24}$$

Assume $g_0^A(\varepsilon_0) = \varepsilon_0$ with distribution $d_0^A(\varepsilon_0)$, $g_u^A(\varepsilon_u) = \varepsilon_u$ with distribution $d_u^A(\varepsilon_u)$, $g_0^B(\varepsilon_0) = \varepsilon_0$ with distribution $d_0^B(\varepsilon_0)$, and $g_u^B(\varepsilon_u) = \varepsilon_u$ with distribution $d_u^B(\varepsilon_u)$.

Suppose the distributions of ε_0 and ε_u for class A are $d_0^A(\varepsilon_0) = \Phi(\frac{\varepsilon_0 - \mu_0^A}{\sigma_0^A})$ and $d_u^A(\varepsilon_u) = \Phi(\frac{\varepsilon_u - \mu_u^A}{\sigma_u^A})$, respectively, where $\Phi(x) = \int_{-\infty}^{x}\frac{1}{\sqrt{2\pi}}\exp(-\frac{1}{2}v^2)dv$ is the distribution function of the standard normal distribution. We may choose some

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Algorithm 2. SLC for binary QEC

Set the index of iterations $k = 0$
Choose a set of arbitrary controls $u^{k=0}(t) = \{u_m^0(t),\ m = 1,2,\dots,M\}, t \in [0,T]$
repeat (for each iterative process)
  repeat (for each member in training subset D_{N_A}, $n_A = 1,2,\dots,N_A$)
    Compute the propagator $U^k_{\varepsilon_0^{n_A},\varepsilon_u^{n_A}}(t)$ with the control strategy $u^k(t)$
  until $n_A = N_A$
  repeat (for each member in training subset D_{N_B}, $n_B = N_A+1, N_A+2,\dots,N$)
    Compute the propagator $U^k_{\varepsilon_0^{n_B},\varepsilon_u^{n_B}}(t)$ with the control strategy $u^k(t)$
  until $n_B = N$
  repeat (for each control $u_m(t)$ $(m = 1,2,\dots,M)$ of the control vector $u^k(t)$)
    $\delta_m^k(t) := \nabla J_N(u_m^k)$ and compute $\nabla J_N(u_m^k)$
    $u_m^{k+1}(t) = u_m^k(t) + \eta_k\delta_m^k(t)$
  until $m = M$
  $k = k+1$
until the learning process ends
The optimal control strategy $u^*(t) = \{u_m^*(t)\} = \{u_m^k(t)\},\ m = 1,2,\dots,M$

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equally spaced samples in the $\varepsilon_0 - \varepsilon_u$ space. For example, we may choose the intervals of $[\mu_0^A - 3\sigma_0^A, \mu_0^A + 3\sigma_0^A]$ and $[\mu_u^A - 3\sigma_u^A, \mu_u^A + 3\sigma_u^A]$, and divide them into $N_{\varepsilon_0}^A + 1$ and $N_{\varepsilon_u}^A + 1$ subintervals, respectively, where $N_{\varepsilon_0}^A$ and $N_{\varepsilon_u}^A$ are usually positive odd numbers. Then the number of samples for class A is $N_A = N_{\varepsilon_0}^A N_{\varepsilon_u}^A$, where $\varepsilon_0^{n_A}$ and $\varepsilon_u^{n_A}$ can be chosen from the combination of $(\varepsilon_0^{n_A^0}, \varepsilon_u^{n_A^u})$ as follows

$$\begin{cases}
\varepsilon_0^{n_A} \in \{\varepsilon_0^{n_A^0} = \mu_0^A - 3\sigma_0^A + \frac{(2n_A^0-1)3\sigma_0^A}{N_{\varepsilon_0}^A},\ n_A^0 = 1,2,\dots,N_{\varepsilon_0}^A\},\\
\varepsilon_u^{n_A} \in \{\varepsilon_u^{n_A^u} = \mu_u^A - 3\sigma_u^A + \frac{(2n_A^u-1)3\sigma_u^A}{N_{\varepsilon_u}^A},\ n_A^u = 1,2,\dots,N_{\varepsilon_u}^A\}.
\end{cases} \tag{25}$$

A similar expression to (25) defines the samples for class B. We use the performance function as defined in (22) with $w_A = w_B = 0.5$. Now we use *Algorithm 2* to find the optimal control strategy.

The parameter settings are listed as follows: $w_A = w_B = 0.5$, the initial state for each member of the quantum ensemble $C_0 = (1,0)^T$, i.e., $|\psi_0\rangle = |0\rangle$, and the target state for members belonging to class A $C_{\text{targetA}} = (1,0)^T$, i.e., $|\psi_{\text{targetA}}\rangle = |0\rangle$; the target state for elements belonging to class B $C_{\text{targetB}} = (0,1)^T$, i.e., $|\psi_{\text{targetB}}\rangle = |1\rangle$; The ending time $T = 8$ (in atomic units) and the total time duration $[0,T]$ is equally discretized into $Q = 800$ time slices with each time slice $\Delta t = (t_q - t_{q-1})|_{q=1,2,\dots,Q} = T/Q = 0.01$; $N_{\varepsilon_0}^A = N_{\varepsilon_u}^A = N_{\varepsilon_0}^B = N_{\varepsilon_u}^B = 5$; the learning rate $\eta_k = 0.2$; the control strategy is initialized as $u^{k=0}(t) = \{u_1^0(t) = \sin t, u_2^0(t) = \sin t\}$.

In the training step, we use $J(u)$ as the performance function which represents the measure of weighted accuracy for QEC. After we apply the optimized control u^* to the inhomogeneous quantum ensemble, we use fidelity to characterize how well every member is classified. The fidelity between the

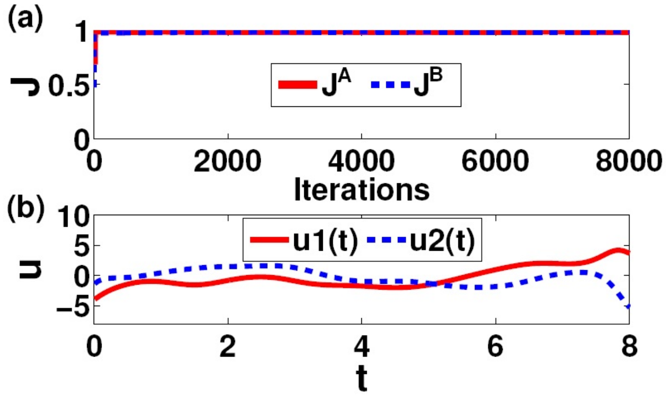

Fig. 3. Learning performance of binary QEC: (a) evolution of performance function J^A and J^B; (b) the learned optimal control for QEC.

final state $|\psi^A_{\varepsilon_0,\varepsilon_u}(T)\rangle$ of a member belonging to class A and the target state $|\psi_{\text{targetA}}\rangle$ is defined as follows [4]

$$F(|\psi^A_{\varepsilon_0,\varepsilon_u}(T)\rangle, |\psi_{\text{targetA}}\rangle) = |\langle\psi^A_{\varepsilon_0,\varepsilon_u}(T)|\psi_{\text{targetA}}\rangle|. \tag{26}$$

A similar representation can be defined for the final state $|\psi^B_{\varepsilon_0,\varepsilon_u}(T)\rangle$ of a member belonging to class B and the target state $|\psi_{\text{targetB}}\rangle$. It is clear that the accuracy of QEC can be calculated with

$$\begin{aligned}\zeta \quad &= J(u) = \tfrac{1}{2}(\mathbb{E}[J^A] + \mathbb{E}[J^B]) \\ &= \tfrac{1}{2}(\mathbb{E}[F^2(|\psi^A_{\varepsilon_0,\varepsilon_u}(T)\rangle, |\psi_{\text{targetA}}\rangle)] \\ &\quad + \mathbb{E}[F^2(|\psi^B_{\varepsilon_0,\varepsilon_u}(T)\rangle, |\psi_{\text{targetB}}\rangle)]).\end{aligned} \tag{27}$$

In the numerical example, we let $\mu^A_0 = \mu^A_u = 0.85$, $\mu^B_0 = \mu^B_u = 1.15$, $3\sigma^A_0 = 3\sigma^A_u = 3\sigma^B_0 = 3\sigma^B_u = 0.05$. The learning control performance is shown in Fig. 3. As shown in Fig. 3, the learning algorithm converges quickly after about 8000 steps of iterations and finds an optimized control for the coherent control step of binary QEC. Applying the learned control to 300 randomly selected testing samples (150 for *class A* and 150 for *class B*), the mean value of fidelity for the testing of *class A* is 0.9976 and for *class B* is 0.9985.

These results show the SLC approach is effective for the binary QEC problem and can achieve a high level of classification accuracy.

V. Conclusions

In this paper, we present a systematic classification approach for inhomogeneous quantum ensembles by combining an SLC approach with quantum discrimination. The classification process is accomplished via simultaneously steering members belonging to different classes to different corresponding target states (e.g., eigenstates). Numerical experiments are carried out to test the performance of the proposed approach for the binary classification of two-level quantum ensembles. All the numerical results demonstrate the effectiveness of the proposed approach for quantum ensemble classification.

Acknowledgment

This work was supported by the Natural Science Foundation of China (Nos.61273327, 61004049 and 61374092), by the Australian Research Council (DP130101658 and FL110100020) and by the US NSF (No. CHE-0718610).

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