Robust Quantum Control in Games: an Adversarial Learning Approach

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High-precision operation of quantum computing systems must be robust to uncertainties and noises in the quantum hardware. In this paper, we show that through a game played between the uncertainties (or noises) and the controls, adversarial uncertainty samples can be generated to train highly robust controls through the search for Nash equilibria (NE). We propose two effective learning schemes, namely the best-response approach and the better-response approach, to make the learning converge faster to robust controls. Numerical experiments demonstrate a remarkable enhancement of control robustness while preserving high accuracy.

PACS numbers:

I. INTRODUCTION

Recent experimental breakthroughs in quantum computing have signaled its commercialization in a foreseeable future [1–3]. To proceed, highly precise and stable control techniques must be developed for deterministic implementation of quantum gates [4]. Generally, high-precision is relatively easy to achieve if a well characterized model is available, for example, using highly efficient GRAPE (gradient ascent pulse engineering) algorithm [5]. The real challenge is to maintain the high precision in presence of realistic uncertainties and noises in the model, i.e., finding both high-precision and robust controls. In the literature, a variety of proposals have been put forward for either online or offline searches for robust quantum controls, e.g., stimulated Raman adiabatic passage working to overcome pulse shape errors [6, 7], dynamical decoupling fighting against decoherence noises [8, 9], and differential evolution [10] as well as ensemble-based algorithms [11, 12] aiming to deal with a variety of noises and uncertainties.

Recently, a class of robust control design methods have been proposed [13–20]. It was shown that, by Montel Carlo sampling of the uncertainties or noises, the GRAPE algorithm can be exploited to effectively improve the robustness against linewidth broadening [16–18], amplitude errors of control fields [17, 18], coupling uncertainty [20], and clock noises [21].

Most of the above approaches are based on improving robustness of a quantum control protocol quantified by the average performance with respect to the system uncertainties or noises to be suppressed. This measure is relatively easy to evaluate and hence to optimize. However, it is not the unique choice, nor necessarily the best. For example, fighting against the worst-case performance was widely adopted in the control of classical systems [22–24], which leads to a class of min-max problems. The optimization with respect to such objective can effectively reduce the risk of failure, which is demanded by the fault-tolerant quantum computation. The worst-case optimization for robust quantum controls was first formulated in the control of molecular systems against noises in ultrafast laser pulses [25], and a theoretical analysis was later done on the robust performance via the Dyson expansion [26]. However, there are very few algorithms for efficiently solving the associated min-max problem. In [27, 28], the $H_{\infty}$ approach was applied to a class of linear quantum systems in the Heisenberg picture. In [29, 30], sequential convex programming (SCP) was proposed for solving the worst-case robust optimization problem in a
single-qubit system, which decomposes the min-max problem into a sequence of convex optimization procedures.

Since the min-max problem can be taken as a zero-sum game between the control and the uncertainties (or noises) that attempt to affect the objective of the quantum system (e.g., state or gate infidelity) in opposite directions, one can introduce game theoretic learning algorithms that seek Nash equilibria (NE). Even if the Nash equilibrium does not exist or is hard to be reached, the robustness of the control can still be enhanced during the learning process. A successful paradigm is the GAN (Generative Adversarial Nets) model in deep learning [32–35] for generative learning tasks, where a large number of applications show that the robustness of the control can still be enhanced during the learning process. A successful paradigm is the GAN (Generative Adversarial Nets) model in deep learning [32–35] for generative learning tasks, where a large number of applications show that the learning model can be trained to be more generalizable by actively generating adversarial samples produced by a discriminator neural network.

In this paper, we will extend this idea to the design of robust quantum controls with respect to the worst-case system disturbance. The remainder of this paper will be arranged as follows. Sec. II presents a game-theoretic analysis of the robust control problem. In Sec. III we introduce several adversarial learning control algorithms based on the dynamic processes in the game theory of learning and evolution. In Sec. IV the effectiveness of the proposed algorithms is illustrated through simulations of the control design in two representative examples. Finally, concluding remarks are made in Sec. V.

II. THE ZERO-SUM GAME BETWEEN CONTROL AND UNCERTAINTY

Consider an $N$-dimensional quantum control system whose unitary propagator obeys the following Schrödinger equation:

$$\dot{U}(t; u, \epsilon) = -iH[t; u, \epsilon]U(t; u, \epsilon)$$

(1)

where $U(\cdot) \in \mathbb{C}^{N \times N}$ represents the quantum gate operation whose initial value is the identity matrix. The system’s Hamiltonian $H[t; u, \epsilon]$ is dependent on a vector of control parameters $u$ (e.g., in-phase and quadrature amplitudes, or phases and amplitudes of laser pulses in the frequency-domain) and a vector of uncertainty parameters $\epsilon$ (e.g., environmental noises or imprecisely identified parameters).

Let $U_f$ be the target gate operation and

$$L[u, \epsilon] = N^{-2}\|U(T; u, \epsilon) - U_f\|^2$$

(2)

be the infidelity of the controlled gate under control $u$ and uncertainty $\epsilon$, where $\| \cdot \|$ is the Frobenius norm. The robustness objective is to find a control $u$ under which $L[u, \epsilon]$ is as small as possible for as many as possible values of the uncertainty $\epsilon$.

A straightforward approach adopted in most existing studies is to minimize the average infidelity, i.e.,

$$E_\epsilon L[u, \epsilon] = \int L[u, \epsilon]p_0(\epsilon)d\epsilon,$$  

(3)

where $p_0(\epsilon)$ is the probability density distribution of $\epsilon$. This objective is relatively easy to estimate and thus to optimize, but the resulting control may not be able to dictate all possible cases of uncertainties due to a lack of control over the variance of the infidelity (i.e., the infidelity can be high over certain small ranges of uncertainties even if the average infidelity is low).

To reduce the risk of encountering high infidelity, we consider the worst-case performance instead of the average performance, which leads to the following min-max problem:

$$\min_u \max_\epsilon L[u, \epsilon]$$

(4)

that does not rely on the probability density distribution of $\epsilon$. Apparently, once the worst-case infidelity is below the desired threshold value, the risk of high infidelity can be effectively reduced.

From a game theoretic point of view, the optimization process can be taken as a zero-sum game between two players, the control $u$ and the uncertainty $\epsilon$, in which $u$ attempts to reduce the gate infidelity while $\epsilon$ tries to increase it. A robust control is thus naturally associated with the NE point $(u^*, \epsilon^*)$ of the game at which each player is unable to go any further by tuning merely $u$ or merely $\epsilon$, i.e.,

$$u^* = \arg \min_u L[u, \epsilon^*] \text{ and } \epsilon^* = \arg \max_\epsilon L[u^*, \epsilon].$$

(5)

A standard approach to search for the NE is to alternately minimize (with respect to $u$) and maximize (with respect to $\epsilon$) the infidelity. The maximization process generates the so-called adversarial samples of $\epsilon$ that yield the worst performance,
against which the control robustness can be gradually enhanced via the minimization processes. In this spirit, a family of learning algorithms can be devised in which the uncertainty parameters play a more active role instead of just being averaged out. Since the gradient-based GRAPE algorithm is always applied in the minimization process, the adversarial learning algorithms to be presented below will be termed as a-GRAPE, where “a” stands for “adversarial”.

It should be noted that the order of actions taken by the two players is not specified in the game, which implies that the solution of the min-max problem (4) with ordered action must be a NE satisfying the condition (5), but a NE may not be a solution of (4). Nevertheless, the NE-gradient optimization can still effectively improve the robustness of controls, and it does not matter whether the solution of (4) is reached or not.

III. THE DESIGN OF ADVERSARIAL LEARNING CONTROL ALGORITHMS

In this section, we will propose two types of a-GRAPE algorithms, namely the best-response and better-response approaches, for training highly robust controls via active selection of adversarial samples.

A. Best-response approach

The simplest NE-seeking approach consists of rounds of alternate optimization with the control and the uncertainty. Suppose that we have obtained an adversarial sample $\varepsilon^{(k)}$ subject to the optimal control $u^{(k)}$ in the $k$-th round. In the $(k + 1)$-th round, we first minimize $L[u, \varepsilon^{(k)}]$ with respect to $u$ using the GRAPE algorithm, which updates the control by $u^{(k+1)}$. Then, we update the adversarial sample of uncertainty parameters by $\varepsilon^{(k+1)}$ that maximizes $L[u^{(k+1)}, \varepsilon]$ with respect to $\varepsilon$.

In terms of game theory, we call such an adversarial learning process a best-response approach because each player chooses its best strategy against the opponent [36]. This learning strategy had been very successful in the training of generative adversarial networks (GANs) for learning the distribution of data [35]. However, for most robust quantum control problems, the best-response strategy can hardly reach a pure NE. This is because such NE requires $L[u^*, \varepsilon] = 0$ for all admissible $\varepsilon$ as the control has adequate resources (e.g., bandwidth) such that $\min_u L[u, \varepsilon] = 0$ for any fixed $\varepsilon$, but this condition is hard to satisfy unless $\varepsilon$ is only allowed to vary over a very small domain. Since a min-max problem possesses NE when the minimization problem is convex and maximization problem is concave, a viable strategy is to seek a mixed NE in an enlarged domain, where the uncertainty $\varepsilon$ is allowed to adopt mixed strategies, i.e., instead of picking a single adversarial sample, we generate a distribution of adversarial samples. Mathematically, this leads to the following min-max problem:

$$
\min_u \max_{p(\varepsilon) \in P} \int L[u, \varepsilon]p(\varepsilon)d\varepsilon,
$$

where the maximization is performed over the space of probability density distributions $P$. The mixed NE is a strategy profile $(u^*, p^*(\varepsilon))$ that satisfies

$$
\begin{align*}
    u^* &= \arg \min_u \int L[u, \varepsilon]p^*(\varepsilon)d\varepsilon, \\
    p^*(\varepsilon) &= \arg \max_{p(\varepsilon)} \int L[u^*, \varepsilon]p(\varepsilon)d\varepsilon.
\end{align*}
$$

The advantage of searching a mixed NE is that their existence is more likely ensured by the linear dependence in $p(\varepsilon)$ and hence a mixed NE is easier to find.

However, problem (6) is computationally much more expensive than problem (4) because the search space for the maximization part is much larger. In practice, this issue can be released by approximating the optimal probability distributions that simplifies the maximization process.

Here, we propose that the optimal distribution $p(\varepsilon)$ can be approximated by exploiting adversarial samples found in the past rounds. Concretely, we perform the maximization process in the same way as the above best-response approach and approximate the optimal probability distribution in the $(k + 1)$-th round as

$$
    p^{(k+1)}(\varepsilon) \approx \frac{1}{k} \sum_{j=1}^{k} \delta(\varepsilon - \varepsilon^{(j)})
$$

using the historic adversarial samples $\varepsilon^{(1)}, \varepsilon^{(2)}, \ldots, \varepsilon^{(k)}$ in the past $k$ rounds. Consequently, in the following minimization process, the objective function based on the distribution,
can be written as the average infidelity over the $k$ adversarial samples

$$J[u, B_k] = \frac{1}{k} \sum_{j=1}^{k} L[u, \epsilon^{(j)}], \quad (8)$$

where $B_k = \{\epsilon^{(1)}, \ldots, \epsilon^{(k)}\}$.

In practice, the approximation (7) can be chosen more flexibly. For example, one does not have to use all historic adversarial samples in (8), because it will be too costly when $k$ is large and elder samples are likely less adversarial. We can keep only the latest few samples, i.e., let the algorithm utilize only a finite number, say $s$, of adversarial samples (see Algorithm 1 for a summary). In this scenario, the original best-response approach can be taken as a special case with memory size being $s = 1$.

**Algorithm 1:** best-response a-GRAPE

**Initialize:**
- a randomly chosen initial control $u^{(0)}$;
- an initial uncertainty sample set $B_0 = \{0\}$;
- a set memory size $s$.

**Repeat:**
1. Use GRAPE algorithm to update the control by the optimal solution of $J[u, B_{k-1}]$, i.e.,
   $$u^{(k)} = \arg \min_u J[u, B_{k-1}],$$
   in which $u^{(k-1)}$ is taken as the initial guess for the GRAPE algorithm. Here, $k$ is an index to the current number of round;
2. Generate a new adversarial sample by
   $$\epsilon^{(k)} = \arg \max_{\epsilon} L[u^{(k)}, \epsilon];$$
3. Update:
   - if $|B_k| < s$, then $B_k = B_{k-1} \cup \{\epsilon^{(k)}\}$,
   - else $B_k = \{\epsilon^{(k)}, \epsilon^{(k-1)}, \ldots, \epsilon^{(k-s+1)}\}$.

**Until** Stopping criteria satisfied.

**B. Better-response approach**

In the above best-response approach, the minimization process is usually efficient as long as the control resource (e.g., bandwidth, time duration, etc.) is abundant, owing to the underlying nice control landscape topology over which almost all locally optimal controls are actually globally optimal [37, 38]. However, the generation of adversarial samples is much harder because the maximization process is usually non-concave. Here, we soften this problem by choosing strongly, but not necessarily the strongest adversarial samples for the training of robust controls. In this regard, we call such method a better-response approach.

The simplest way to search for better-response adversarial samples is to randomly choose a batch of uncertainty samples, calculate their corresponding cost, and keep the worst few ones among them for the adversarial training in the next round (see Algorithm 2 for a description). The batch size of the samples should be sufficiently large so that the chosen adversarial samples are close to the worst-case samples, but not too large to maintain computational efficiency. Naturally the better-response approach relying on random sampling usually takes more rounds of gaming, but each round can be much faster when the batch is not very large. Moreover, the randomness of sample batches in the better-response approach may bring additional benefits for the search to get away from unwanted false worst-case traps.

**Algorithm 2:** better-response a-GRAPE

**Initialize:**
- a randomly chosen initial control $u^{(0)}$;
- a set ratio $r$, $r \in (0, 1)$.

**Repeat:**
1. Randomly generate $M$ uncertainty samples, compute the corresponding infidelity and form an adversarial sample set denoted as $B_k$ by retaining the first $rM$ worst ones, where $k$ denotes the current number of round;
2. Use GRAPE algorithm to update the control by
   $$u^{(k)} = \arg \min_u J[u, B_k];$$

**Until** Stopping criteria satisfied.

**IV. SIMULATION RESULTS**

To illustrate the above game-based adversarial learning strategies, we simulate two quantum gate synthesis examples in this section.
Fig 1: The learning curves of a-GRAPE for robust control of a two-qubit system. The red curves correspond to the worst-case infidelity while the blue ones correspond to minimized average infidelity over selected adversarial samples in cases (a) the best-response approach with memory size $s = 10$ and (b) the better-response approach with $M = 100$ and $r = 0.1$.

A. Two-qubit system

Consider a two-qubit quantum gate control problem with the following system Hamiltonian:

$$H(t) = (1 + \epsilon_0)g\sigma_{1z} \otimes \sigma_{2z} + \sum_{i=1}^{2}(1 + \epsilon_i) \cdot [u_{ix}(t)\sigma_{ix} + u_{iy}(t)\sigma_{iy}],$$

where $g = 10$ MHz is the identified qubit-qubit coupling strength with $\epsilon_0$ being the identification error in the coupling constant; $\epsilon_1$ and $\epsilon_2$ represent the inhomogeneity of control fields. The dimensionless three uncertainty parameters are all assumed to be bounded by $|\epsilon_i| \leq 0.2$. In the simulation, the time duration of control pulses is chosen as $T = 300$ ns, which is evenly divided into $M = 100$ intervals over which the control fields are piecewise constant. The target gate $U_f$ is set as the controlled-NOT gate.

In the best-response approach, we apply a genetic algorithm to seek adversarial samples, and use 10 historic adversarial samples to train the control function in each round. In the better-response approach, we uniformly generate $M = 100$ random uncertainty samples in each round and keep the first 10% (i.e., $r = 0.1$) worst ones as adversarial samples for training the control. Figure 1 shows the resulting learning curves, namely the achieved worst-case infidelity $L_{\text{max}}$ versus the number of rounds, as well as the corresponding minimized average infidelity $J_{\text{min}}$ over the selected adversarial samples versus the number of rounds. The robustness of the controls can be directly witnessed from the curves of worst-case infidelity, which are all enhanced during the optimization. The $L_{\text{max}}$-curve is initially far apart from the $J_{\text{min}}$-curve, but the gap is quickly reduced after several rounds of gaming. In the best-response approach, the gap is almost closed, showing that the optimized control and uncertainty samples is likely close to a mixed NE. In the better-response approach, the gap still remains large after 2000 rounds. For both approaches, the control robustness is still enhanced by the game, with the (approximate) worst-case infidelity decreased to the level of $10^{-2}$.

As discussed above, neither the average performance nor the worst-case performance is the unique measure for quantifying the control robustness. To better evaluate the overall performance of an optimized control, we calculate and display the cumulative probability distribution function (cdf) $F(l)$ of the gate infidelity, i.e., the probability for the infidelity being not greater than $l$, in Fig. 2. Here, we also compare the a-GRAPE algorithms with our recently proposed b-GRAPE algorithm [20] (see Appendix for details) for robust control design subject to the average infidelity (i.e., Eq. (3)). In the simulations, the b-GRAPE algorithm is run with 1 million iterations having the mini-batch size $n_{mb} = 1$ and a learning rate $\alpha = 0.002$, while the a-GRAPE algorithms are run by 20 rounds in the best-response approach and 1504 rounds in the better-response approach. The cdf curve can be used to evaluate the control robustness from two perspectives. On one hand, given a desired value of gate infidelity $l_0$ (e.g., the threshold error for quantum error correction), the cumulative probability $F(l_0)$ gives the confidence that the control can suppress the error below the value $l_0$. On the other hand, given an expected confidence $F_0$ (say, 90%), the cdf can tell us at which threshold value (i.e., $l_0$ such that
$F(q_0) = F_0$ the control can guarantee the confidence. As will be seen below, the robustness performance may vary at different levels of desired infidelity or expected confidence.

Figure 2 clearly shows that the controls optimized by the a-GRAPE algorithms, especially in the better-response approach, are much more robust as almost the entire cdf curve is high above that generated with b-GRAPE algorithm (i.e., with greater confidence at each value of infidelity). For examples, as seen in Tab. I, the control optimized with better-response a-GRAPE can suppress the gate error below $10^{-3}$ with a high confidence 82.5%, while the control optimized with b-GRAPE has only 43.1% confidence. At the higher-precision level (i.e., infidelity lower than $10^{-4}$), the better-response approach still maintains 34.2% confidence, while the control optimized with b-GRAPE provides almost zero confidence. The performance of the best-response a-GRAPE is only a little poorer than b-GRAPE in high-precision regime, but much higher in low-precision to medium-precision regime (i.e., infidelity in $10^{-2}$, $10^{-3}$). Besides, consistent with the findings in Fig. 3, the best-response a-GRAPE achieves a low worst-case infidelity than that achieved by the better-response a-GRAPE. However, the best-response a-GRAPE has poorer performance in high-precision regime than the better-response a-GRAPE, as can be also indicated by the $J_{\min}$ curves displayed in Fig. 3, from which it can be also observed that the best-response approach can ensure a lower worst-case infidelity as indicated by the $L_{\max}$ curves. The comparison between different algorithms shows that there is no unique criterion for evaluating the control robustness. An optimized control may achieve a satisfiable precision (e.g., infidelity in $10^{-2}$, $10^{-3}$) over a large regime of uncertainties, but the highest precision it can achieve may be poor. In practice, one needs to balance between the precision and the robust region using limited control resources.

![CDF Curve Comparison](image)

**Table I:** The upper two rows list the confidence for the gate infidelity to be below $10^{-3}$ and $10^{-4}$. The lower two rows list the gate infidelities below which 99% and 80% confidence can be guaranteed.

| Infidelity | b-GRAPE | best-response | better-response |
|------------|---------|---------------|-----------------|
| $10^{-3}$  | 43.1%   | 41.9%         | 82.5%           |
| $10^{-4}$  | 3.7%    | 0.9%          | 34.2%           |
| 99%        | 0.0107  | 0.0033        | 0.0041          |
| 80%        | 0.0043  | 0.0019        | 0.0008          |

**B. Three-qubit system**

To see more clearly how the control performance relies on the uncertainties and algorithmic parameters, we simulate a three-qubit system with two uncertainty parameters, whose Hamiltonian is as follows

$$H(t) = J_{12}(1 + \epsilon_1)\sigma_1\sigma_2 + J_{23}(1 + \epsilon_2)\sigma_2\sigma_3 + \sum_{k=1}^{3} [u_{kx}(t)\sigma_{kx} + u_{ky}(t)\sigma_{ky}],$$

where the nominal coupling constants $J_{12} = J_{23} = 10$ MHz. The uncertainty parameters $\epsilon_1$ and $\epsilon_2$ (i.e., identification errors of the coupling constant) are bounded by $|\epsilon_i| \leq 0.2$. In the simulation, the target unitary operation is selected as the Toffoli gate. The time interval $[0, T]$, where $T = 1 \mu$s, is evenly divided into $M = 100$ intervals, over which the control fields are piecewise constant.

It has been clear that the controls optimized by a-GRAPE algorithms could improve the worst-case performance, and here we want to see how the performance depends on the parameters, e.g., $s$ and $r$. We first compare the best-response a-GRAPE optimization processes with different memory sizes $s = 1, 10, 15$. The learning
Fig 3: The worst-case infidelity versus the number of rounds in best-response a-GRAPE optimization of the three-qubit system with different memory size.

curves are shown in Fig. 3 in which the minimization curves are not displayed because the worst-case performance is only related with the maximization curve. It can be seen that the algorithm converges faster and finds more robust controls when using more, but not too many, historic adversarial samples. For example, the worst-case infidelity reaches $10^{-2}$ after only 7 rounds when $s = 10$, which converges faster than the case $s = 1$, and the worst infidelity is much lower. However, the case $s = 15$ performs more poorly than the case $s = 10$. This is reasonable because elder historic samples tend to be less adversarial due to the fading memory effect.

For the better-response approach, we choose $M = 100$ and compare the performance under $r = 0.01$, 0.05, and 0.1, where the true worst-case infidelity in each round is estimated by 2000 independent random samples. Similarly to the case of the best-response approach, simulation results (see the learning curves in Fig. 4) show that the robustness of the optimized controls can be improved by using adequately many adversarial samples, but too many of them will not bring further improvement.

Since there are only two uncertainty parameters in this example, we can plot a 3D landscape to show how the infidelity varies with them, from which we can evaluate the overall robustness. In Fig. 5, we display 3D plots under controls optimized with b-GRAPE (after 2 million iterations), best-response a-GRAPE (after 629 rounds) and better-response a-GRAPE (after 1986 rounds) algorithms. The comparison shows that both a-GRAPE algorithms outperform the b-GRAPE algorithm as most of their landscape surfaces are below that of b-GRAPE. The best-response a-GRAPE achieves the lowest worst-case infidelity and effectively suppresses almost the entire landscape down below the level of $L = 10^{-3}$. However, its overall performance in higher-precision regimes (e.g., $L = 10^{-4}$) is poorer than the better-response a-GRAPE.

In addition to the best-response and better-response approaches, the a-GRAPE algorithms can be designed more flexibly (i.e., relaxed) such that they still work efficiently when the uncertainty vector $\epsilon$ is of large scale. For example, we may also perform the minimization process in a better-response manner. As is described in Algorithm 3, we may update the control by only a few gradient-descent iterations (or stop at some prescribed error threshold) without having to reach the ultimate minimum, which responds better but not best to the adversarial sample. The maximization part can be done either with best-response or better-response approaches. In this regard, the SCP algorithm [31] can be considered as a special case of the relaxed better-response approach with fixed sampled uncertainties and carefully selected learning rates.

To assess the feasibility of this idea, we apply relaxed best-response (with $s = 5$, $n = 20$ and


Fig 5: The infidelity versus uncertainty parameters under controls optimized with b-GRAPE with $n_{rob} = 1$ and $\alpha = 0.002$, best-response dynamic with memory size $s = 10$, better-response approach with ratio $r = 0.05$ respectively.

$m = 20$) and better-response (with $r = 0.25$, $n = 30$ and $m = 20$) a-GRAPE algorithms to the same three-qubit example. As is shown in Fig. 5, where the control robustness is evaluated by the cumulative probability functions, the relaxed a-GRAPE algorithms can also greatly outperform the b-GRAPE algorithm. Comparing with their unrelaxed counterparts, the relaxed best-response and better-response a-GRAPE algorithms are not only faster, but also more robust in high-precision regime (e.g., near the infidelity level $10^{-4}$).

**V. CONCLUSION**

We have proposed a family of adversarial learning algorithms, including best-response and better-response approaches, for robust control design of quantum systems. The algorithms are subject to the minimization of worst-case gate infidelity, which can be treated and resolved from a game-theoretic perspective. Numerical simulations show that these a-GRAPE algorithms can achieve high control robustness. In particular, the best-response approach can effectively suppress the error over a larger domain at a satisfiable level of precision, but in extremely high-precision regime, the better-response performs better. Both approaches have their practical applications depending on the specific requirement of the control. We also demonstrate that the family of a-GRAPE algorithms can be expanded by choosing better-response strategies in both the maximization and minimization processes.

It should be noted that, although a-GRAPE usually performs better than b-GRAPE, the computational burden is also heavier, and the tuning of algorithm parameters (e.g., memory sizes, batch size).

**Algorithm 3: relaxed best/better-response a-GRAPE**

**Initialize:**
- a randomly chosen initial control $u$;
- a set memory size $s$ or ratio $r$;
- an initial adversarial sample set $B$.

**Repeat:**
1. Randomly generate $m$ uncertainty samples, and select the worst one or the first $rm$ worst ones;
2. Do the following GRAPE optimization for $n$ iterations:
   $$ u \leftarrow u - \alpha \cdot \frac{\delta}{\delta u} J[u, B]. $$
   Here, $\alpha$ represents the learning rate;
3. Update the adversarial sample set $B$ as described in Algorithm 1 or 2;

**Until** Stopping criteria satisfied.

Fig 6: The cumulative probability versus infidelity under the corresponding controls used in Fig. 5 and the ones obtained from the relaxed best-response approach run by 10995 rounds and the relaxed better-response algorithm run by 3850 rounds.
sizes, ratios or learning rates) are application specific. How to optimize the choices of these parameters, or even in an adaptive fashion, will be an important target for future studies.

As we remarked in Sec. III, we did not require on the existence of Nash equilibria (NE) as the algorithm can enhance the robustness no matter whether the NE exists or not. From our simulations, it appears that a mixed NE is more likely approached in the best-response a-GRAPE with larger memory size. From a theoretical perspective, a better understanding of the potentially existing NE will be still useful. This will be explored in future studies.

Acknowledgments

This work is supported by the National Key R&D Program of China (Grants No. 2017YFA0304304) and NSFC (Grants No. 61833010 and No. 61773232).

Appendix: b-GRAPE algorithm

The b-GRAPE algorithm presented in [20] is a stochastic gradient algorithm. The optimization process follows the gradient evaluated with randomly chosen batches of samples, so that the uncertainties can be effectively used to improve the robustness. Here, “b” stands the “batch”. The b-GRAPE algorithm is described in Algorithm 4.

Algorithm 4: b-GRAPE

Initialize:
a randomly chosen initial control \( u^{(0)} \);
an initial momentum \( v^{(0)} = 0 \);
a set minibatch size \( n_{mb} \);
Repeat:
(1) Randomly select a subset \( S_k \) of the uncertainty sample with \( |S_k| = n_{mb} \), where \( k \) denotes the current number of round;
(2) Update the control by
\[
   u^{(k)} = u^{(k-1)} + v^{(k)},
\]
where
\[
   v^{(k)} = \lambda v^{(k-1)} - \frac{\alpha}{n_{mb}} \sum_{\epsilon \in S_k} \frac{\delta}{\delta u} L[u^{(k-1)}, \epsilon].
\]
Here, \( \alpha \) represents the learning rate and the weight parameter \( \lambda \) is chosen to be 0.9 in this paper;
Until Stopping criteria satisfied.
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