Machine-learning assisted quantum control in random environment

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Disorder in condensed matter and atomic physics is responsible for a great variety of fascinating quantum phenomena, which are still challenging for understanding, not to mention the relevant dynamical control. Here we introduce proof of the concept and analyze neural network-based machine learning algorithm for achieving feasible high-fidelity quantum control of a particle in random environment. To explicitly demonstrate its capabilities, we show that convolutional neural networks are able to solve this problem as they can recognize the disorder and, by supervised learning, further produce the policy for the efficient low-energy cost control of a quantum particle in a time-dependent random potential. We have shown that the accuracy of the proposed algorithm is enhanced by a higher-dimensional mapping of the disorder pattern and using two neural networks, each properly trained for the given task. The designed method, being computationally more efficient than the gradient-descent optimization, can be applicable to identify and control various noisy quantum systems on a heuristic basis.

I. INTRODUCTION

Machine learning (ML), which enables computers to learn automatically from available task-specific data [1–4], is revolutionizing modern approaches in physical sciences [5]. In quantum science, ML becomes useful and powerful [6] in particle physics, many-body physics [7], and quantum computing [8] among others. Recently developed learning architectures [9] such as convolution neural networks (CNN), having a considerable success in object detection and image classification, were beneficial to classify phases of matter [10], study nonequilibrium glasses [11], find hidden order in electronic-quantum-matter imaging data [12] and identify the thermodynamic time arrow [13].

All the above studies were performed for systems where disorder is either nonexistent or plays a negligible role in the system dynamics. In practice, impurities, noise, and other imperfections are ubiquitous and unavoidable in condensed matter [14] and its simulated counterparts [15]. Particularly, the ultracold atoms offer a feasible and controllable platform for studying the disorder [16–19]. In this scenario, the random potential is implemented by optical means, and brings for studying the disorder [16–19]. In this scenario, the random potential is implemented by optical means, and brings about a variety of intriguing phenomena [20–24], i.e. localization effects, phase transitions, and superfluidity, due to the interplay among the disorder, nonlinearity, trapping potential or/and spin-orbit coupling. Along with these developments, the power of supervised learning (SL) is harnessed to categorize stochastic data, extract quantitative information from this data, and predict the features of complex quantum systems, at a reasonable computational cost [25–30].

However, quantum control under disorder still remains a major challenge [31–35], though optimal control [36–38], ML [25, 39–42], and shortcuts to adiabaticity [43, 44] have been exploited for fast manipulations in regular systems. The extensive study of stochastic systems [45, 46] have emerged in quest for controlling the dissipative dynamics most efficiently. However, when it comes to disorder, to classify or identify stochastic data embodied in the dynamics is a conundrum. As the size of the stochastic sample increases dramatically, the higher power of ML is demanding in such complexity.

To work out this problem, we establish the ML approach for identifying and controlling dynamics of a quantum system with disorder. For this purpose, we use deep learning with two CNNs for high-fidelity control of a quantum particle in a time-varying trapping potential embedded in random environment. We begin with an important result: training the CNN can efficiently preselect the relevant type of the disorder realization from tens of thousands of stochastic samples. Then, we introduce the second CNN to find the optimal control policy such as the time-dependent potential shape, in a training regression model. To make the optimization more efficient, the randomness classification from deep learning is an essential pretraining for disordered system under control, thus removing the redundant data. Thus, the SL with CNNs provides the ability to generalize the tasks beyond their original design, applicable to any realization of random potential. Our methods pave an efficient way for the robust optimal control, i.e. cooling, transporting, trapping atoms or charged particles (ions and electrons) [39, 43, 47], by taking into account environmental noise and randomness.

II. DISORDERED SYSTEM AND CONTROL STRATEGY

Consider a quantum particle of mass $m \equiv 1$, located at the sum of time-dependent harmonic potential and a random potential of impurities. The corresponding Hamiltonian (with $\hbar \equiv 1$) reads

$$H(t) = \frac{p^2}{2} + \frac{1}{2}\omega^2(t)x^2 + U_r(x),$$

where $p$ is the momentum, $\omega(t)$ is the frequency of harmonic trap, and $U_r(x)$ is the random potential of interest. Equation (1) describes atoms in optical traps and electrons in acoustic
The shift in the ground state energy as impurities position, respectively.

\[ \omega \]

The frequency modulation, i.e. from we are using the system of units with \( t \). FIG. 1. Probability densities of the initial (\( t = 0 \), black solid line) and final (\( t = t_f \), black dashed line) ground states in the harmonic trap in the random environment forming the total potential \( U(x) \). Two realizations are presented to illustrate the effect of disorder. The corresponding final states (blue dotted lines) produced by the optimal control policy with SL are shown as well. The total initial (red solid line) and final (red dashed line) potentials, are also shown for the eye. Parameters: \( U_0 = 1, \omega_0 = 1, \) and \( \omega_j = 0.1 \). Here and below we use \( \xi = d = 1/8 \) for \( N = 160 \) impurities at the \((-10, 10)\) interval. Since we are using the system of units with \( h \equiv m \equiv 1 \), the length and the energy are measured in the units of \( 1/\sqrt{\omega_0} \) and \( \omega_0 \), respectively.

Traps [47] and gate-formed quantum dots. The motivation behind the frequency modulation, i.e. from \( \omega(t \leq 0) = \omega_0 \) to \( \omega(t = t_f) = \omega_f \), is to achieve the fast high-fidelity expansion/compression within a short time \( t_f \), beyond the adiabatic criteria [39, 43].

We study generic random potential \( U_r(x) \), corresponding to the Anderson-like disorder, produced by the disorder-free harmonic potential. The parameters \( \omega_0 = 1, \omega_f = 0.1, t_f = 1, \) and \( \Omega = \sqrt{\omega_0} \), taken here as an example. Interestingly, for a given set \( A = \{a_1, a_2\} \) the fidelity in the presence of disorder can be higher than that for the disorder-free harmonic potential. The parameters \( a_1 \) and \( a_2 \) are measured in the units of \( \omega_f^2 \) and \( \omega_f^2 \), respectively. Note that behavior of \( \omega^2(t) \) in (b) is counterintuitive since it includes a considerable increase at \( t \) close to \( t_f = 1 \).

and obtain \( \ell \sim (U_0 \xi/\sqrt{d})^{2/3} \) with the corresponding energy \( \epsilon_{\text{loc}} \sim (U_0 \xi/\sqrt{d})^{4/3} \). Therefore, in the parabolic potential, localized states can be located at the distances up to \( w_d \sim \sqrt{\epsilon_{\text{loc}}/\omega} \sim (U_0 \xi/\sqrt{d})^{2/3}/\omega \), meaning that the decrease in \( \omega \), the ground state can be positioned at a large distance from the origin.

Figure 1 illustrates that the eigenstates of the final trap can be completely changed by different realizations of random potential, as compared to the disorder-free results. For the realization in Fig. 1 (b), where the initial and final states are almost orthogonal, the high-fidelity results cannot be achieved even with the optimal control policy presented below. This intriguing feature makes the previous methods [39, 43] invalid in our current problem. As a consequence, we need improved statistical analysis and computational method.

To prove the principle of ML application we choose the third-order polynomial

\[ \omega(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3, \]

as the control function for the trap frequency, where \( a_0 = \omega_0 \), and \( a_1 = [\omega_f - (\omega_0 + a_1 t_f + a_2 t_f^2)]/t_f^2 \) are given by the boundary conditions, \( \omega(0) = \omega_0 \) and \( \omega(t_f) = \omega_f \). The initial state at \( t = 0 \) is assumed to be the ground state for simplicity. The freedom left in \( a_1 \) and \( a_2 \) offers the possibility to optimize the control function \( \omega(t) \), thus finding the maximum ground-state fidelity defined as

\[ F \equiv \int_{-\infty}^{\infty} \psi^*(x, t_f) \psi_{\text{gr}}(x) \phi_{\omega_f} dx, \]

where \( \psi_{\text{gr}}(x) \phi_{\omega_f} \) is the ground state in the random potential corresponding to \( \omega_f \), and \( \phi(x, t_f) \) is obtained by a direct numerical solution of the non-stationary Schrödinger equation.
with the Hamiltonian $H(t)$ from Eq. (1). The optimal design of the trap frequency through the control policy $A = \{a_1, a_2\}$ can produce $\psi(x, t_f)$ with the maximum possible fidelity.

We impose two conditions on the optimal control function, with the hint from the analysis on the high-fidelity control without disorder in Appendix A. First, it has to provide a high fidelity for the quantities of interest, in this case, as defined in Eq. (4). Second, $\omega^2(t)$ should correspond to a moderate energy consumption required for the transition, suggesting that the maximum $\omega^2_{\text{max}}(t)$ does not exceed a certain value $\Omega^2$ such that the process is experimentally feasible. Figure 2 illustrates the high-fidelity zone control policy $A = \{a_1, a_2\}$ and corresponding feasible control function $\omega(t)$, satisfying the criteria $\omega^2_{\text{max}}(t) \leq \Omega^2 = 6$. The search for the optimal coefficients in the relevant $\{a_1, a_2\}$ range (see Fig. 2) is a time-consuming task even for a given realization. Since the stationary state and dynamics rely on the disorder realizations, the optimization of control policy also requires immense computing power. Note that the total number of disorder realizations in Eq. (2) is approximately $2^N$. However, in agreement with the manifold hypothesis [48], many of these realizations produce similar $U_i(x)$-functions with similar $\psi_i(x, \omega_j)$ width and positions. Therefore, the ML can use databases of moderate ($\leq 10^5$) size. In what follows, we are motivated to develop the SL based on two CNNs to overcome such challenge.

III. MACHINE LEARNING PROCEDURE

Now, we proceed to use SL, comprising two CNNs, for classifying the disorder realizations and constructing the optimal control policy, through the connection between the random sequence $S_i[j]$ and the optimal control policy $A_{\text{opt}}$, see the schematic diagram in Fig. 3. One can refer to Appendix B for the technical description of SL.

First, we generate $4 \times 10^4$ disorder realizations with the labeled sequences $S_i[j]$ as the inputs. For each realization, the fidelity of overlap between the eigenstates at $t = t_f$ and final wavefunctions resulting from the state evolution [see Eq. (4)] is numerically calculated with the control function $\omega(t)$ in Eq. (3). The maximum fidelity for the given $i$–the realization, $F^\text{max}_i$, and corresponding control policy $A_i$ are thus determined by using the same approach in Fig. 2, where the criteria $\Omega^2 = 6$ and $F_i = 0.9$ are applied to bound the feasibility and fidelity, while keeping a considerable size of database. The whole database $X = \{S_i, F^\text{max}_i, A_i\}$ is finally established, where 80% of the database is selected as a training set, and the rest as a testing set.

Then, we introduce the first CNN, named in what follows CNN1, in deep learning to assign each given realization of the random potential to a set of classes, for instance, whether it determines feasible high-fidelity (FH) or not. Such randomness recognition is classification, aiming at selecting the reasonable inputs of realizations. To be more efficient, we extend the input $S_i[j]$ into two-dimensional (2D) grid (see Appendix B.2) before the neural network is trained, by converting each sequence $S_i[j]$ into a two-dimensional (2D) matrix $S_i^{[2D]}[j_1, j_2]$ by using

$$S_i^{[2D]}[j_1, j_2] \equiv S_i[j_1] + S_i[j_2].$$

As expected, the randomness recognition based on 2D grid surpasses the one-dimensional (1D) one, in the sense that the accuracy of classification and loss of regression are improved at the cost of computation time. Therefore, we use $S_i^{[2D]}[j_1, j_2]$ as the inputs and $y_i$ as the output, where FH ($y_i = 1$) and anti-FH ($y_i = 0$) suggests the aforementioned criteria, $F > F_b = 0.9$ and $\omega^2_{\text{max}}(t) \leq 6$, is satisfied or not.

For classification in the CNN1 we employ the standard sequential structure (convolution and pooling layers), and choose the loss function as $L_i(y, p) = -\sum_i\log(p_i)$, with $p_i$ being the probability produced by network, and the accuracy $N_r/N$, with $N_r$ being the number of the right predictions out of total $N$. After using optimizer Adam() at the rate of $10^{-4}$, we manage to select 5886 out of $4 \times 10^4$ realizations, with the accuracy above 97%, see Fig. 4 (a) and the relative portion of the selected realizations being of the order of the $w_{eb1}/w_{d1} \sim \omega^1_{\text{max}}/(Uo\xi/\sqrt{D})^{2/3}$ ratio, where $w_{eb1}$ is taken at $t = 0$. Obviously, this pretraining process is critical for classifying the disorder and excluding realizations yielding the low-fidelity control, as shown in Fig. 1 (b). Remarkably, the high efficiency of CNN1 can be conceptually interpreted by comparing its feature-map with the corresponding position of final wave packet, also see the detailed discussion in Appendix C.2.

Next, to find the optimal control policy $A_{\text{opt}}$, we construct the second CNN (CNN2) for regression. We choose the loss function $L_2(y, \hat{y}) = \sum(y_i - \hat{y}_i)^2/N$, where $y$ and $\hat{y}$ are the actual and predicted results of control policy $A$. The residual neural network [49] is used in CNN2, with a shortcut channel. We define fidelity deviation of each realizations $\Delta F_i = |F^\text{max}_i - F'_i|$ with $F'_i$ being the fidelity predicted by control policy. During the training process, we further define the average value over each $N$-sized batch $\Delta F = \sum_{i=1}^{N} \Delta F_i/N$ in every training epoch for quantifying the performance of CNN2. As a consequence, we train the CNN2 for achieving $\Delta F \leq 10^{-4}$, see Fig. 4 (b). Thereby, during the process we record the loss at each batch and the fidelity of predicted policies, and finally obtain the trained CNN1 and CNN2, as indicated by solid lines in Fig. 4 (a, b). Moreover, we produce 100 realizations for verifying the performance of trained CNNs in
FIG. 4. The accuracy of CNN1 (a) and the fidelity deviation (b) are displayed for classification and regression, where the dashed and solid lines represent the average value of test and training batches in each epoch. The shadow area indicates the value distribution of batches. (c) The fidelity deviation from two trained CNNs are presented for 100 testing realizations of random potential.

FIG. 5. The average accuracy in CNN1 (a) and the average fidelity deviation in CNN2 (b) for the last ten epochs are illustrated for different $\omega_f$ and $t_f$, where the structure and hyperparameters are the same as those in Fig. 4, and the error bars represent their deviations.

IV. DISCUSSION

There are several points to be addressed on the generality of our proposed method. We can, in principle, choose other $\omega(t)$ ansatzes with more parameters or even use the results from the gradient-descent optimization. The detailed analysis clarifies that the influence of the form of ansatz (or moderate changing in the bound $F_b$ and/or $\Omega$) on the classification of disorder, performed by the CNN1, is essentially negligible, since the border line between high and low fidelity is mostly determined by the intrinsic property such as the shape of the disorder rather than by the external condition. However, malfunctioning or poor performance of CNN1 can cause low efficiency of CNN2, obtaining the input from CNN1. The ansatz (3) serves as a reference for setting the criteria. Note that the CNNs trained with the gradient-descent optimization is not better than the ones with such simple ansatz, see the detailed discussion in the Appendix C1.

Moreover, we can also apply the trained CNNs to different values of $t_f$ and $\omega_f$. Figure 5 indicates the average accuracy in CNN1 and the average fidelity deviation in CNN2 for the last ten epochs by using the same structure and hyperparameter as before. On the one hand, when $\omega_f$ is increased, the random realizations are much easier to recognize, thus resulting in higher accuracy. It makes sense that the influence of random potentials on the fidelity can be negligible, when the trap potential is strong enough to localize the state near the origin. However, the more realizations as the inputs of CNN2 finally lead to the larger fidelity deviation as shown in Fig. 5. On the other hand, according to the time-energy trade-off, larger $t_f$ (still far away from the adiabaticity) increase the area corresponding to condition $\omega_f^2(t) \leq \Omega^2$ (cf. Fig. 2). Thus, more random realizations corresponding to the feasible $A_{\text{opt}}$ increase the statistical uncertainty and degrade the performance of trained CNNs. That is, the fidelity deviation in CNN2 becomes larger because of worse classification, depending on the distribution and number of the selected realizations in CNN1, see Fig. 5. In a word, the combined effects of the trapping potential and disorder plays an important role in dynamical control, characterized by the fidelity and the required energy cost, e.g. the laser power for optical trap or the electrical power for quantum dots.

V. CONCLUSIONS

The behavior of quantum objects such as atoms and charged particles in random potentials is an active research area, with a lot of the accumulated knowledge and even more yet unknowns. The complexity prevents the researchers from efficiently controlling the quantum dynamics in random environments. We presented a remedy by developing proof-of-principle supervised learning algorithms, trained through deep neural networks, to classify the randomness and find the optimal control policy. The efficiency and accuracy of the pro-
posed algorithm is based on using two-dimensional mapping of the random potential and sequential application of two neural networks, each trained for the given different task. Our results indicate that machine learning, based on the convolutional neural network for classification and regression, can be used to control various quantum systems with impurities, noise and imperfections, and ultimately to unveil the physical insight into the interplay of disorder and quantum dynamics. With the advent of techniques of configurable optical traps [50] and surface acoustic waves [51, 52], we suggest the experimental verification of the proposed method for trapped atoms or electrons in random environment.

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Appendix A: high fidelity quantum control without disorder

To begin, we consider the case without random potential, $U_r(x) \equiv 0$, in order to have a reference for understanding the effects induced by the disorder. By setting $m \equiv 1$ and $h \equiv 1$, the Hamiltonian of a single particle trapped in a harmonic potential reads

$$H = \frac{p^2}{2} + \frac{1}{2} \omega^2(t)x^2,$$

(A1)

which describes the compression and decompression by tailoring the frequency $\omega(t)$ of the harmonic trap. According to the Lewis-Riesenfeld invariant theory, the solution of time-dependent Schrödinger equation admits analytical expression [43]:

$$\psi(x, t) = \left(\frac{\omega_0}{\pi b^2}\right)^{1/4} \exp\left[-\frac{i}{2} \int_0^t \frac{\omega_0}{b^2} dt'\right] \exp\left[i \frac{1}{2} \left(\frac{\tilde{b}}{b} + \frac{i \omega_0}{b^2}\right)x^2\right],$$

(A2)

where the auxiliary function $b(t)$ satisfies the Ermakov equation:

$$\tilde{b} + \omega^2(t)b = \frac{\omega_0^2}{b^3}.$$  

(A3)

For a decompression process from the initial frequency $\omega_0$ to final frequency $\omega_f$, the boundary conditions can be formulated as $b(0) = 1$, $b(t_f) = \gamma$ ($\gamma = \sqrt{\omega_0/\omega_f} > 1$), $b(0) = \dot{b}(t_f) = 0$. Thus, for an arbitrary control function $\omega(t)$, we are able to calculate the time-dependent scaling parameter of $b(t)$ and corresponding $\dot{b}(t)$ by solving the Ermakov equation. By considering the ground state, with the initial and final boundary conditions, we, in general, can reach the ideal target state, that is, $\psi_p(x|\omega_f) = (\omega_0/\pi \gamma^2)^{1/4} e^{-\omega_0 x^2/2 \gamma^2}$. Based on Eq. (A4), the fidelity can be analytically expressed as

$$F = \left[\frac{4 \omega_0^2 \gamma^2}{\omega_0^2 (\gamma^2 + b_f^2)^2 + (b_f \gamma^2)^2}\right]^{1/2},$$

(A4)

where $b_f = b(t_f)$ and $\dot{b}_f = \dot{b}(t_f)$ are the numerical solution of Eq. (A3) at $t = t_f$. Obviously, the fidelity $F$ strongly depends on $b_f$ and $\dot{b}_f$. When $b_f = \gamma$ and $\dot{b}_f = 0$, we will have $F = 1$. In this case, we recall the concept of shortcuts to adiabaticity, that is, to achieve fast adiabatic-like decompression without final excitation.

Without loss of the generality, we choose the simple ansatz $\omega(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$, such that the fidelity is calculated, depending on the coefficients $a_1$ and $a_2$. To understand the performance of the fidelity, Fig. 6 (a) and (b) illustrate the dependence of $b(t_f)$ and $\dot{b}(t_f)$ on $\{a_1, a_2\}$, respectively. Figure 6 (c) finally shows the plot of the fidelity dependent of the coefficient set $A = \{a_1, a_2\}$, in which the stripes occurs due to the interplay between $b(t_f)$ and $\dot{b}(t_f)$. The high-fidelity regime in Fig. 6 gives the criteria for machine learning later, when the random potential is involved.

Appendix B: machine learning

Machine Learning (ML) methods, including support vector machines, decision trees, random forests and artificial neural networks (ANNs), have been developed in last decades. Moreover, the deep learning is proposed to handle the huge quantity of data and complex system, notably, the ANNs is usually outperform than others. Nowadays, the ANNs are dedicated to solving complex tasks such as the image and video recognition, analysis of strategical games (AlphaGo), etc. In particular, the deep convolutional neural networks (CNNs), initially proposed for computer vision learning, now are overwhelming in the artificial intelligence (AI) industry. Their unique architecture, inspired by research on the brain’s visual cortex, greatly enhances the performance of analysis of systems in complex surroundings, which is consistent with our problem on quantum control in a random environment.

The reasons for using the CNNs to analyze the disordered system are three-fold: (1) Data grows exponentially with
tremendous amount of disorder realizations; (2) Training an ANN can be accelerated by using graphic processor units (GPUs); (3) CNN can be used to identify the disorder as the application in image classification.

Next, we shall exploit the supervised learning, based on two CNNs, for classifying and controlling the joint effect of a regular (parabolic) potential and disorder.

1. neural network and supervised learning

A deep ANN consists of input, hidden and output layers, and the depth of network usually depends on the amount of hidden layer. Meanwhile, a single layer is composed by a set of nodes, and each node is connected with the others from the next layer with a particular weight and bias. Moreover, the learning process of ANNs is combined by the forward-propagation and back-propagation computation based on the gradient descent algorithm. We start with the propagating data from the input layer, pass the hidden layer(s), measure the output layer, and finally calculate network error based upon the network predictions. With the error function and the gradient-base optimizer, the back-propagation decreases error by updating the weights and bias of network. Compared with a regular ANNs, the CNNs are trained to optimize the filters (or kernels) through the automated learning, instead of the hand-engineered in feature extraction. It takes advantage of the hierarchical pattern in capturing data feature and reducing the number of the parameters involved. In order to explain the functioning of this CNN, we shall make use of the following notation:

1. \( x' \) is the data flow of \( \ell \)th layer.
2. The filter \( K \) with the size \( k_1 \times k_2 \) has \( m \) and \( n \) as the iterators.
3. The weight between \( \ell \) layer and \( \ell - 1 \) layer is represented by \( \omega' \), and the corresponding bias \( b' \).
4. \( f(\cdot) \) is an activation function.
5. The underlying data of layer is \( x'_\ell = \sum_{m,n} \sum_{j} f(w_{m,n}x'_{\ell-1} + b'_j) \), where \( i \) and \( j \) are the iterator.
6. \( x' \otimes K^k \) represents the data extracting process by the \( k \)th filters.
7. \( y_i \) and \( y'_i \) are the actual and predicted values (labels), respectively.

Supposing that we use \( k \) filters, the output of \( \ell \)-th convolutional layer can be presented as

\[
x'_{i,j} = \sum_{k=0}^{k} x'^{\ell-1}_{i,j} \otimes K^k = \sum_{k=0}^{k} \sum_{m,n} f(k^k_{m,n}x'_{\ell-1} + b'),
\]

where the activation function \( f(\cdot) \) is the logistic Sigmoid function, \( f(z) = 1/(1 + \exp(-z)) \), or the rectified linear unit (ReLU) function, \( f(z) = \max(0,z) \). The Sigmoid function maps the data from \([-\infty, \infty]\) into \([0,1]\), resulting in the probability of prediction as the output of network. And the ReLU is a piecewise step function, \( \text{ReLU}(x) = \max(x, 0) \), that transfers the input data from \([-\infty, \infty]\) into \([0, \infty]\). Such two nonlinear activation functions are widely used to allow the nodes to learn more complex structures in the data. A pooling layer, aiming to reduce the spatial size, contains \text{MaxPooling()} and \text{AveragePooling()}. More specifically, they extract the maximum (or average) value of the pooling block from the previous layer, thus reducing the amount of the parameters. The CNN layer is schematically shown in Fig. 7, in which we set the \(16 \times 16\) inputting data and three \(7 \times 7\) filters for the convolution layer and three \(2 \times 2\) filters for calculating the maximal pooling.

Next, we introduce the loss function and gradient-based optimizer for classification and regression. Regarding the classification task, the loss function is defined as the following cross-entropy form:

\[
J(W, b; y, y') = \frac{1}{N} \sum_{i=1}^{N} J_1(W, b; y_i, y'_i),
\]

with

\[
J_1(W, b; y_i, y'_i) = -y_i \log \left[ \sigma(y'_i) \right],
\]

where \( W \) is the weight collection of network for \( N \) samples, and \( \sigma(y'_i) \) is the softmax probability, where the Softmax function \( \sigma(z) = e^z/(\sum_j e^j) \) is used for normalizing the output. As for the two-category image classification \( k = 2 \) task, the input layer is a flatten pixel sequence \( x_i \) of image, and the result is the probability of labels. For instance, when the actual binary label is \( y_0 = \{1, 0\} \), and two dimension output \( y'_0 = \{p_0, p_1\} \), the error for a single prediction thus is \( j = -y_0 \log[y'_0]^T \). On the other hand, for the regression process, the loss function in (B2) is a mean squared error:

\[
J_2(W, b; y, y') = \sum_{i} |y_i - y'_i|^2,
\]

which represents the deviation from the regression prediction \( y'_i \) to the actual sample \( y_i \). We use the optimizer \text{Adam()}, which is included in the application programming interface (API) of PyTorch, for optimizing the loss function in the learning process. Back-propagation (or forward pass) refers to the calculation and storage of the intermediate variables (weights and bias) of a neural network, and minimizes the cost function.
by gradient-based optimizer. This can be simply expressed as

\[
\text{Repeat : } \left\{ W_{i,j}^{t} = W_{i,j}^{t-1} - \eta \frac{\partial \mathcal{L}}{\partial W_{i,j}} \right\}, \qquad (B5)
\]

with learning rate \( \eta \).

Following that, we create the algorithm for our task, which consists of two CNNs for classification and regression, respectively. We encode the algorithm based on the PyTorch [53] software platform, where the deep learning library consists of the tensor flow and the computation is accelerated by GPUs. In order to illustrate the learning algorithm, we briefly introduce the functions that we used in the PyTorch API:

1. **2D convolution layer**
   \( \text{Conv2d (inchannel, outchannel, kernel size, stride)} \).
2. **Max pooling layer** \( \text{MaxPool2d (kernel size)} \).
3. **ReLU** and **Sigmoid** represent the rectified linear unit function and the corresponding logistic function, respectively.
4. **CrossEntropyLoss** and **MSELoss** indicates the loss function of Eqs. (B2) and (B4).

The variables include: **inchannel**: the depth of channel in the input, **outchannel**: the number of output channel depends on the amount of filter (or kernel), **kernel size**: the filter size, **stride**: controlling the stride for the cross-correlation.

The detailed parameters can be further found in the PyTorch tutorial [53]. Along with this user-friendly platform, we now construct the algorithm for the supervised learning. Before proceeding, we should design the architecture of CNN1 and CNN2, since the performance of a neural network mostly depends on its structure and layer depth. According to the complexity of task, the architecture of CNN1 is built up as a standard sequential network and CNN2 as a ResNet network [54], see the details in the flow chart in Fig. 8. The residual block **Residual()**, with so-called “identity shortcut connection”, skips two layers, as shown in Fig. 8. It makes the network possible to train hundreds layers, keeping the compelling performance. After introducing the CNNs-based supervised learning and the architecture of two networks, we can start with creating the database and training the model for classification and regression.

![FIG. 8. Diagrammatic architectures of CNN1 and CNN2, are illustrated, where the function and its parameters are presented for each layer of network and the residual block of CNN2 in the dashed frame is specified. More details can be found in the main text.](Image)

![FIG. 9. (a) Dependence of the maximum value of \( \omega^2(t) \) on the coefficient set \( \{a_1, a_2\} \), and the white dashed curve presents the contour of \( \omega^2(t) = 6 \). (b) The proportion of four classifications, based on two criteria \( F > F_b \) and \( \omega^2_{\text{max}}(t) \leq \Omega^2 \), in the prepared database as the function of \( F_b \). The distribution of maximum fidelity \( F_{\text{max}} \) for 400 exemplified realizations is plotted in (c), and one of realization in 2D grid is illustrated in (d). Here the criteria \( F_b = 0.9 \) and \( \Omega = \sqrt{6} \) are used, and other parameters as the same as those in Fig. 6.](Image)

2. **classification and regression**

For supervised learning, two essential steps, including data preparation and model training, are required. In this sense, the performance of model can be improved by increasing the training data and selecting a high-quality database. To calculate the database, however, is a time-consuming task for a complex system, so it is significant to preselect for producing a representative database with high quality. Let us consult the Fig. 1 of the main text, in which the eigenstates of the final trap can be completely changed by different realizations of random potential, and some of them will result in the low-fidelity control for sure. Thus, we propose CNN1 for the preselection, in order to establish the link between input and output data of network by choosing a small amount of high-quality database. We will demonstrate that the high-quality database not only brings the benefits to training process, but also makes the trained network more universal and tolerant.

Aiming to present the feature of each single random sequence, we initially extend the one-dimension (1D) sequence in two-dimension (2D) grid, see Eq. (5). More specifically, as in the main text, we select a \( 1 \times 160 \) random sequence, e.g., \( S_i[j] = \{1, 1, -1, 1, ..., -1, 1\} \). A typical resulting 2D grid with the elements 2,0, and \(-2\), is shown in Fig. 9 (d). We will see the advantage of 2D \( S_i^{[2D]}[j_1, j_2] \) as the input data, in the following discussion.

Next, we generate \( 4 \times 10^4 \) realizations of disorder, and thus calculate the maximum fidelity \( F_{\text{max}} \) and the corresponding policy \( A_j \) of \( 200 \times 200 \) coefficient grid in the range of
Here we set two conditions for the optimal control function. First, it has to provide a high fidelity for the quantities of interest, i.e., $F_{\text{max}} > F_b$. Second, the corresponding $\omega^2(t)$ should correspond to a moderate energy consumption required for the transition, implying that $\omega^2_{\text{max}}(t)$ has not exceeded a certain value $\Omega^2$. In practice, by taking into account the experimental constraints, such as the limited laser intensity or the gate field in quantum dots, we set the control policy, $\omega^2_{\text{max}}(t) \leq \Omega^2$, where we take $\Omega = \sqrt{6}$ as the critical value for defining “feasible” policy. In Fig. 9 (a), the contour curve for $\omega^2_{\text{max}} = 6$ is presented. Moreover, the optimal policy $A_{\text{opt}}$ is constrained by these two conditions: $F_{\text{max}} > F_b$ and $\omega^2_{\text{max}}(t) \leq \Omega^2$ (labeled by FH). The ratio of the database as a function of $F_b$ is also presented in Fig. 9 (b), from which we find that the amount of FH database is decreased when we set larger bound, $F_b$, for the fidelity. Obviously, the disorder effect makes the fidelity worse, though the higher fidelity is desirable in the quantum control in the presence of random environment. In order to keep balance between the amount of high-fidelity realizations and the diversity of database, we set the bound $F_b = 0.9$ as the criteria for keeping the reasonable database, see Fig. 9 (c). With the assistance of the prepared database satisfying such criteria, we shall discuss the network and training process as follows.

Previously, we attempted to find the regression between $S_i^{[2D]}[j_1, j_2]$ and $A_{\text{opt}}$ by using only one CNN. However, the results are not reasonable, and a very complex neural network is required to provide the expressibility and universality for the variety of disorder realization. Nevertheless, we create an intuitive scheme to reduce the complexity of database, that is, the classification is added prior to the regression. The database is divided into two categories by the pretraining process: the realization satisfying feasible high-fidelity (labeled FH) criteria or not (labeled anti-FH). As a consequence, the database for regression is firstly filtered by the classification (CNN1) process based on two aforementioned criteria, and secondly train the network (CNN2) based on previously identified FH database.

Now, we train the CNN1 with the input $X = S_i^{[2D]}[j_1, j_2]$ and output $Y = \{0, 1\}$ by selecting the loss function $\text{CrossEntropyLoss}(\cdot)$ respect to Eq. (B2). The identified FH database from CNN1 is the input data of CNN2, and the output is optimal policy $A_{\text{opt}}$ with the loss function $\text{MSELoss}(\cdot)$ in Eq. (B4). Two architectures of CNNs are presented in Fig. 8, where there are 7 layers in a regular sequential network CNN1 and 34-layer ResNet34 [54] for CNN2. Meanwhile, we use the optimizer Adam [55] to optimize the parameters based on the gradient descent algorithm. Moreover, we define the accuracy $N_c / N$ (with $N_c$ being the number of the right predictions out of total $N$) for CNN1, which is the correct prediction number over the total amount of database. Meanwhile, for quantifying the result of regression, we also define the fidelity deviation $\Delta F = |F_{\text{max}}^i - F_i^j|$, where $F_{\text{max}}^i$ is the actual maximum fidelity and $F_i^j$ is the numerical result from the policy predicted by the network (as in Sec. III of the main text).

To this end, we formulate the training algorithm as

**Algorithm 1:** Training CNN for classification/regression

Input: The database $\{x, y\}$
Output: Trained CNN initialization;
optimizer=Adam(learning rate = 0.0001);
$loss = \text{CrossEntropyLoss}(\cdot)$ (or $\text{MSELoss}(\cdot)$);

while epoch do
for batch in range(epoch size) do
    net.train();
predictions = net($x_i[\text{batch}]$);
    training loss = loss(predictions, $y_i[\text{batch}]$),
    optimizer(net),
total loss += training loss,
end

end

3. machine learning outcome

In this section, we present a detailed training process and further discuss the results. To proceed with the training and testing, we choose the parameters, such as $\omega = 1$, $\omega_f = 0.1$, and $t_f = 1$. The coefficients in the control function of $\omega(t)$ are in the range of $a_1 \in [-30, 30]$ and $a_2 \in [-100, 100]$, and the classification criteria are $F_b = 0.9$ and $\Omega = \sqrt{6}$. The whole database $X = \{S_i, F_{\text{max}}^i, A_i\}$ for $4 \times 10^4$ realizations in the $200 \times 200$ coefficient grid are established by a 50-core computer for more than 10 hours. The input data for CNN1 is a 2D random grid $x_i = \{S_i[2D]\}$ and the output is $y_i = \{0, 1\}$, to classify the optimal policy is FH ($y = 1$) or anti-FH ($y = 0$). Remarkably, CNN1 manages to select 5886 realizations out of $4 \times 10^4$, when the criteria, $F > F_b = 0.9$ and $\omega^2_{\text{max}}(t) \leq \Omega^2 = 6$, are stipulated. Eventually, we convert these classified realizations into the CNN2 as the input database, and the corresponding optimal policy $A_{\text{opt}}$ is obtained as the output data. For both two networks, 80% of input database is the training database and the rest testing part. One can find other parameters in Fig. 8 and more details in the code.

It turns out that the accuracy of CNN1 can reach 97% after 30 iterations (epochs = 30), and the fidelity deviation for CNN2 is below than $10^{-4}$ after 50 iterations (epochs = 50). The average loss of training and testing data are presented by the solid and dashed curves in Fig. 10 (a, b), where we see that the overfitting occurs at 10 epoch for classification, and at 20 epoch for regression.

After that, we shall discuss the generality of our method and the tolerance of model for changing the hyperparameters. First of all, we compare the performance of two trained CNNs by using 1D and 2D input data. The accuracy and fidelity deviation $\Delta F$ for 1D and 2D input data are presented in Fig. 10 (c, d), where Conv1d() and Conv2d() are exploited for 1D and 2D cases, and the rest parameters are same. It is evident that the model using 2D input data outperforms the 1D model.
To this end, we prepare the databases of 1, and (c) $f_0$, $\omega_0$, $t_1$, and (d) $f_0$, $\omega_0$, $t_1$, $t_2$ are considered. By comparison, the larger potential is strong enough such that the localized state has to be located near the origin. Consequently, the lower loss of CNN1 is achieved since the most of disorder realizations are much easier to recognize, when the final trap frequency is $\omega_2$. In Fig. 11, we specify the maximum fidelity located in the whole database for the various conditions. The restriction imposed by $\Omega = \sqrt{6}$ is illustrated by black dashed curve in (a, b, c). The other parameters are the same as those in Fig. 6.

in terms of accuracy and fidelity deviation.

Second, we elaborate the generality of our training model by checking the performance with various values of $\omega_f$ and $t_f$. To this end, we prepare the databases of $1.6 \times 10^4$ realizations for $t_f = \{1, 2, 3, 4\}$ and $\omega_f = \{0.2, 0.4, 0.6, 0.8\}$, the criteria and parameters of two CNNs are the same as previous case when $t_f = 1$, $\omega_f = 0.1$. In Fig. 11, we specify the maximum fidelity located in the whole database for the various conditions, where (a) $\omega_f = 0.1$, $t_f = 1$, (b) $\omega_f = 0.4$, $t_f = 1$, and (c) $\omega_f = 0.1$, $t_f = 2$ are considered. By comparison, the larger $\omega_f$ results in the higher fidelity, since the random realizations are much easier to recognize, when the final trap frequency is increased. This is due to the fact that the influence of random potentials on the fidelity can be negligible, when the final trap potential is strong enough such that the localized state has to be located near the origin. Consequently, the lower loss of CNN1 is achieved since the most of disorder realizations are labeled as FH, on the contrary, more inputs causes the performance of CNN2 to degrade. In addition, according to the time-energy trade-off, the increase of total time $t_f$ makes the designed trap frequency easier to satisfy the predetermined criteria ($F > F_h = 0.9$ and $\omega_{\text{max}}(t) \leq \Omega^2 = 6$), yielding the larger area in Fig. 7 (c). In this case, the database is difficult to recognize, see Fig. 11, since more random realizations corresponding to the feasible $A_{\text{opt}}$ increase the statistical uncertainty and degrade the performance of trained CNNs. Therefore, the loss of CNN1 becomes larger when the total time $t_f$, but the loss of CNN2 decreases conversely. All these results are consistent with those of accuracy and fidelity deviation in Fig. 5 of main text. Clearly, the quantity and quality of the database determine the performance of CNNs, depending on the physical constraints or conditions, or the total time, the amplitude of disorder, and trapping potential. More important, we conclude that the interplay of the trapping potential and disorder is of critical significance for controlling the dynamics in terms of the fidelity and the required energy.

Finally, we check the performance of the deep CNNs in terms of the hyperparameter, such as the number of hidden layers, the size and number of filters, etc. In our model, the depth of the CNN2 is much larger than that of CNN1, which suggests that the CNN2 is more sensitive to the hyperparameters. For simplicity, we concentrate on two hyperparameters, the filter number and hidden layers, in the CNN2. In this network, the first layer's outchannel number is $N_f$ (see Fig. 8), which determines the total number of filters. With different $N_f = [4, 8, 16, 32]$, we compare the average loss of testing data for 10-layer ResNet10, 18-layer ResNet18, 34-layer ResNet34, and 50-layer ResNet50. The clear dependence on these hyperparameters is presented in Fig. 12 (a, b), in which the corresponding average training and testing losses of the last ten epochs are calculated by using same parameters, respectively. Obviously, the expressibility of network depends on the number of parameters. The average training loss decreases when the number of layers or filters increases. However, we emphasize that the over-fitting of the network appears when the network complexity (the number of nodes and alternative paths) increases, see Fig. 12 (b). Here we note that all calculations are implemented by using the online computa-
tion resource from the Google’s cloud service called ‘Colab’, which contains GPUs acceleration. For 30 epochs, it takes about 300 seconds for training the CNN1, but more than \(10^3\) seconds for the CNN2 while calculation of the fidelity deviation \(\Delta F\) takes several hours. The suggested algorithm can be realized at a regular computer without GPU’s acceleration albeit with a much longer computation time.

**Appendix C: discussions**

1. **Gradient-descent optimization**

Here we discuss the generality of the ansatz used here in our proposed method. One might be interested to try other ansatz and even optimal (or near-optimal) approach, combined with ML. Regarding the latter, a powerful numerical tool, for example, the gradient-descent (GD) algorithm can be applied directly, not as a working tool of the ML algorithms. To clarify the advantages and disadvantages of this approach, let us study the possible trade-off on the improvement of fidelity in the problem of interest and the ability of training CNNs. Thus, we compare the optimal solutions produced by GD with the polynomial ansatz-based results.

A parametric optimization problem is the minimization of a given cost-function by gradient descent. The optimal solution \(M^{\text{opt}}\) can be produced by minimizing cost-value \(c = J(M)\), which can be expressed as:

\[
M^{\text{opt}} = \min_c J(M).
\]  

(C1)

In our scenario, the control function is the trap frequency, \(f(t) = \omega(t)\), with \(N_t\)-intervals discrete time \(t \in [0, t_f]\) (keeping the same \(t_f = 1\) as that in main text). Accordingly, the control tuple \(f(t) = (f(0), f(dt), ..., f(t_f))\) is constrained by \(f(t) \leq \Omega = \sqrt{6}\) and satisfies boundary conditions, e.g. \(f(0) = 1\) and \(f(t_f) = 0.1\). Then, we shall optimize the \(N_t\)-size tuple \(f(t)\) for approaching the highest fidelity by minimizing the infidelity \(1 - F\), in the context of parametric constrained minimization problem. In this regard, we perform the optimization process by algorithm SLSQP [56] based on the scipy platform. For one typical realization of random potential, the GD takes several minutes for searching the optimal control function which satisfies the convergent condition \(|dJ/dM| < 10^{-7}\) of the cost function while our two-step supervised learning method produces the near-optimal solution in several seconds. Next, we are concerned about the efficiency of training two CNNs by using GD-produced databases.

To this end, we calculate the GD-based control function for the same \(4 \times 10^4\)-realization database used in the main text. It is expected that the GD method with \(N_t = 100\) improves the fidelity. Thus, it increases the number of FH realizations, thus providing 6801 of them against 5886 for ansatz-based method. In Fig. 13 we present the fidelity distribution of 500 realizations in (a) for two methods: GD (red circle) and ansatz-based (black cross). More distinctly, we compare 69 realizations among 500, which admit the high fidelity for both methods in (b) of Fig. 13, with the corresponding 69 optimal solutions produced by GD illustrated in (c). One can see that, although the GD-based method slightly increases the fidelity compared to the ansatz-based one, it does not change the fidelity distribution strongly. This result can be understood by the physics argument that the fidelity of control policy de-
depends mainly on the localization induced by random potential rather than on the control strategy. Figure 14 further demonstrates the performance of CNN1 (classification) and CNN2 (regression) trained by the two databases generated from a simple ansatz (blue solid) and GD (black dashed). In addition, one can see the disadvantages of GD-based optimal control as the database for training CNN2. The GD method indeed boosts the fidelity of control policy on the cost of losing the generality in CNN2. It is due to the fact that the performance of GD-based CNN2 is worse: the database dimension $N_t = 100$ is much larger than that for the ansatz-based database (which is 2), eventually decreasing the reliability of the regression process. Thus, the balance between the fidelity improvement and the ability to train the CNN should be kept as our method.

2. **Interpretability of CNNs**

It is difficult to explain the results obtained from ML in an intuitive way, despite of many successful applications in quantum physics [1, 10]. In order to understand the machine-making decision in solving the optimal control problem, we discuss the interpretability (or explainability) of a ML task. The interpretability in ML is defined, for example, by Miller [57]: ‘Interpretability is the degree to which a human can understand the cause of a decision’ or, similarly, by Kim [58] as: ‘Interpretability is the degree to which a human can constantly predict the model’s result’. The interpretability of a training model brings criteria such as comprehensibility, reliability, and fairness of facts upon the process of ML. In a recent work [59], Molnar offers a comprehensive review on
the concept, principles and importance of explainable models in the field of ML. Among them, we offer here the evidence of interpretability by visualizing the feature-map of CNN1 for understanding and explaining the ML outcomes [59].

First, we recall the element of output from the convolution operation Conv2d() :

$$x'_{i,j} = \sum_{m,n} k^k_{mn} x'_{i+m,j+n} + b^j, \quad (C2)$$

where the \(l\)-th feature-map \(x'_i\) is the sum of product of filters \(K_{mn}\), and corresponding filter-size \((l-1)\)-th feature-map \(x'_{i+m,j+n}\) with bias \(b^j\). According to the structure of CNN1 designed in Fig. 8, we have sixteen \(7 \times 7\) weight matrices (filters) in each convolution layer. In Fig. 15, we present 16 parametric filters of last layer in (a) and corresponding bias in (e), and produce 16 feature-maps for three selected realizations in (b-d) after Sigmoid function. For illustration, we extract the most representative feature-maps (labeled by black dashed squares) out of 16 in (e-h) of Fig. 15, and compare them with the corresponding density of the final wavepacket with the trap frequency \(\omega(tf) = \omega_f\). By performing the 4-layer convolution product operation, an original input 2D random grid (see Fig. 9) is transformed into a particular feature map, which can be interpreted by the localization of the target state density. More specifically, the feature-map is strongly correlated with the localization of density for low-fidelity realization, such as (e) and (g) in Fig. 15. For the high-fidelity case, the feature-map is much more uniformly distributed compared to the low-fidelity counterparts. In Fig. 16, we further compare the final state probability density and feature-map for 12 realizations including low-fidelity (a-b) and high-fidelity (b-d) realizations. To this end, one can’t precisely identify the random sequence just by watching the feature-map, in particular, for realizations with \(F \approx 1\) or \(F \rightarrow 1\) can be easily identified and explained, according to the typical feature-map in (e-g) of Fig. 15. It should be emphasized that our results can be interpreted based on the comparison of the feature-map and the wavepacket density. In a word, the accurate ML outcome captures the hints from the feature-maps, which are related to the nature of the localization physics in random potentials.

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