

Approximation of quantum control correction scheme using deep neural networks

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We study the functional relationship between quantum control pulses in the idealized case and the pulses in the presence of an unwanted drift. We show that a class of artificial neural networks called LSTM is able to model this functional relationship with high efficiency, and hence the correction scheme required to counterbalance the effect of the drift. Our solution allows studying the mapping from quantum control pulses to system dynamics and then analysing the robustness of the latter against local variations in the control profile.

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I. INTRODUCTION

The main objective and motivation of quantum information processing is the development of new technologies based on principles of quantum mechanics such as superposition and entanglement [1]. Quantum technologies require the development of methods and principles of quantum control, the control theory of the quantum mechanical system [2]. Such methods have to be developed by taking into account the behaviour of quantum systems. In particular, as quantum systems are very susceptible to noise, which may influence the results of the computation, the methods of quantum control have to include the means for counteracting the decoherence [3].

The presented work is focused on the development of tools suitable for analysing the relation between the control pulses, used for idealized quantum systems, and the control pulses required to execute the quantum computation in the presence of undesirable dynamics. We focus on quantum dynamics described by the quantum spin chain. We are interested in a method of approximating the correction function of normal control pulses (NCP), *i.e.* the function accepting control pulses corresponding to the system without the drift Hamiltonian and generating the de-noising control pulses (DCP) for the system with the drift Hamiltonian. We propose an approximation that not only incorporates the global features of the function but also describes its local properties. This feature is in contrast with available methods based on optimisation which do not take into account the continuous behaviour of the map from NCP to the de-noising control pulses.

Recently, significant research effort has been invested in the application of machine learning methods in quantum information processing [4–6]. In particular, optimization techniques borrowed from machine learning have been used to optimize the dynamics of quantum systems, either for quantum control [7] and simulation [8], or for implementing quantum gates with suitable time-independent Hamiltonians [9]. These techniques include also quantum control techniques from dynamic optimization [10] and reinforcement learning [11]. On the level of gate decomposition, neural networks have also been applied to the problem of decomposing arbitrary operations as a sequence of elementary gate sets [12].

In this paper, we study the correction scheme between control pulses obtained in the ideal case, and the pulses taking into account the undesired dynamics in the system. We propose a method based on an artificial neural network (ANN) for the approximation function of correction scheme, which allows us the analysis of its local properties. Moreover, we demonstrate that the utilized network has high efficiency and reproduces the properties of the model.

This paper is organized as follows. In Section II we introduce the model and describe the architecture of a deep neural network which will be used as an approximation function. In Section III we demonstrate that the proposed methods can be used for generating control pulses without the explicit information about the model of a quantum system. We also utilize it for the purpose of analysing the properties of the correction scheme. Section IV contains summary of the presented results.

II. METHODS: MODEL AND SOLUTION

In this section, we provide necessary notation and background information. We start by introducing a spin-chain model and describe the problem of generating quantum control pulses that counteract the undesired dynamics present in the system. We also introduce the architecture of the artificial neural network used to approximate the correction scheme.

A. Model of quantum system

Let us consider a system of two interacting qubits. The evolution of the system is described by Schrödinger equation

$$\frac{d|\psi\rangle}{dt} = -iH(t)|\psi\rangle \quad (1)$$

where the Hamiltonian has three components

$$H(t) = H_c(t) + H_0 + H_\gamma. \quad (2)$$

We consider the control Hamiltonian of the form

$$H_c(t) = h_x(t)\sigma_x \otimes \mathbb{1} + h_z(t)\sigma_z \otimes \mathbb{1}, \quad (3)$$

and the base Hamiltonian

$$H_0 = \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z. \quad (4)$$

The last element in Eq. (2) is the drift Hamiltonian, which can be an arbitrary two-qubit Hamiltonian multiplied by real parameter $\gamma > 0$.

Quantum optimal control refers to the task of executing a given unitary operation via the evolution of the system, in our case described by Eq. (2). To achieve this, one has to properly choose the coefficients $h(t) = (h_x(t), h_z(t))$ in Eq. (3). The set of reachable unitaries can be characterized [2] by studying the Lie algebra generated by the terms in Eq. (2). For $H_\gamma = 0$ our system is *fully-controllable*, so any target can be obtained with suitable choice of $h(t)$, with no restriction on the control pulses. We assume that function $h(t)$ is piecewise constant in time slots $\Delta t_i = [t_i, t_{i+1}]$, which are the equal partition of evolution time interval $T = \bigcup_{i=0}^{n-1} \Delta t_i$. We also assume that $h_x(t)$ and $h_z(t)$ have values from interval $[-1, 1]$.

Function $h(t)$ will be represented as vectors of values of $h_x(t)$ and $h_z(t)$. For the case $\gamma = 0$, we say that it represents NCP— *normal control pulses*. Alternatively, for $\gamma \neq 0$, we say that $h(t)$ represents

DCP—*de-noising control pulses*. Since $h(t)$ is piecewise constant, both NCP and DCP have two indices, with first index corresponding to time slots $\{0, \dots, n-1\}$, and the second index corresponding to values of control pulses controls $\{x, z\}$, namely

$$\begin{aligned} NCP_{i,j} &= h_j(t), \quad \gamma = 0, \\ DCP_{i,j} &= h_j(t), \quad \gamma \neq 0, \end{aligned} \quad (5)$$

where

$$t \in [t_i, t_{i+1}] \quad i \in \{0, \dots, n-1\}, \quad j \in \{x, z\}. \quad (6)$$

It is worth noting that the mapping from the set of control operations to the unitary operator is not injective. Namely the same unitary can be obtained using different choices of $h(t)$. To study the relationship between NCP and DCP we need to select the DCP which is more closely related to the NCP. Because of continuity, we do that numerically by using the NCP as starting guess of the DCP. The final optimal DCP is then found using a local optimisation around the initial NCP.

The figure of merit in our problem is the fidelity distance between superoperators, defined as [13]

$$F = 1 - F_{err}, \quad (7)$$

with

$$F_{err} = \frac{1}{2N^2} (\text{Tr}(Y - X(T))^\dagger (Y - X(T))), \quad (8)$$

where N is the dimension of the system in question, Y is superoperator of the fixed target operator, and $X(T)$ is evolution superoperator of operator resulting from the numerical integration of Eq. (1) with given controls. In particular, for unitary operator U , its superoperator S is given by the formula

$$S = U \otimes \bar{U}. \quad (9)$$

B. Architecture of artificial neural network

The control pulses used to drive the quantum system with Hamiltonian from Eq. 3 are formally a time series. This aspect suggests that one may study their properties using methods from pattern recognition and machine learning [14, 15] that have been successfully applied to process data with similar characteristics. The mapping from NCP to DCP share similar mathematical properties with that of statistical machine translation [16], a problem which is successfully modelled with artificial neural networks (ANN) [17]. Because of this analogy, we use ANN as

the approximation function to learn the correction scheme for control pulses. A trained artificial neural network will be used as a map from NCP to DCP

$$\text{ANN}(\text{NCP}) = \text{nnDCP}, \quad (10)$$

where nnDCP, neural network DCP, is an approximation of DCP obtained by using the neural network.

Because of time series character of control sequences, we utilize bidirectional long short-term memory (LSTM) networks [18]. The long short-term memory block is a special kind of recurrent neural network (RNN), a type of neural networks which has directed cycles between units. Similarly to other RNN, LSTM networks can take into account hidden states from their history. In the other words, the output in given time depends not only on current input but also on earlier inputs. Therefore, this kind of neural networks is applicable in situations with time series with long-range correlations, such as in natural language processing where the next word depends on the previous sentence but also on the context.

Basic architectures of RNN are not suitable for maintaining long time dependences, due to the so-called *vanishing/exploding gradient problem* – the gradient of the cost function may either exponentially decay or explode as a function of the hidden units. The LSTM unit has a structure specifically built to solve the vanishing/exploding gradient problem of other RNN and is adjusted to maintain memory over long periods of time. The bidirectional version of LSTM is characterized by the fact that it analyses the input sequence/time series forwards and backwards, so it uses not only information from the past but also from the future [19, 20].

For two-qubit systems, we found that three stacked bidirectional LSTM layers are sufficient for obtaining the high value of fidelity. Moreover, at the end of the network, we use one dense layer which processes the output of stacked LSTM to obtain our nnDCP. Experiments are performed using TENSORFLOW library [21, 22].

III. RESULTS: EXPERIMENTS

For the purpose of testing the proposed method we use a sample of random unitary matrices [23]. Pseudo-uniform random unitaries can be obtained also in the quantum control setting via random functions $h(t)$, provided that the control time T is long enough [24]. In our experiments we use QuTIP [25–

27] to generate training and testing data. First, we construct the target operators

$$U \otimes \mathbf{1}, \quad (11)$$

where $U \in U(2)$ is a random matrix. Next, using QuTIP we generate NCP corresponding to the target operators. In the case of our setup, the parameters are fixed as follows:

- time of evolution $T = 6$,
- number of intervals $n = 32$,
- control pulses in $[-1, 1]$.

We train the network using a subset of the generated pairs $\{(\text{NCP}, \text{operator})\}$, and next test it with the complement of the set of pairs.

A. Performance of the neural network

The first experiment is designed to analyse the efficiency of the trained network in terms of fidelity error of generated nnDCP control pulses. Trained LSTM have mean fidelity on the test set as follows:

| H_γ | γ | | | |
|---|----------|------|------|------|
| | 0.2 | 0.4 | 0.6 | 0.8 |
| $\sigma_y \otimes \mathbf{1}$ | .954 | .947 | .929 | .914 |
| $0.2\sigma_x \otimes \mathbf{1} + 0.8\sigma_y \otimes \mathbf{1}$ | .973 | .950 | .924 | .958 |
| $0.4\sigma_x \otimes \mathbf{1} + 0.6\sigma_y \otimes \mathbf{1}$ | .982 | .959 | .944 | .948 |
| $0.6\sigma_x \otimes \mathbf{1} + 0.4\sigma_y \otimes \mathbf{1}$ | .988 | .970 | .956 | .963 |
| $0.8\sigma_x \otimes \mathbf{1} + 0.2\sigma_y \otimes \mathbf{1}$ | .993 | .984 | .968 | .965 |

However, it should be noted that, despite the fact that the mean fidelity on the test set is high, the trained network sometimes has outlier results *i.e.* it returns nnDCP which corresponds to the operator with high fidelity error.

The performed experiments show that it is possible to train LSTM networks for a given system with high efficiency. We trained artificial neural networks on different kinds of drift, *i.e.* $\alpha\sigma_x \otimes \mathbf{1} + (1-\alpha)\sigma_y \otimes \mathbf{1}$ for $\alpha \in \{0, 0.2, 0.4, 0.6, 0.8\}$, with different values of γ . The experiment with this kind of drift is representative because σ_y is orthogonal to the controls σ_x, σ_z . The performed experiment shows that it is possible to train LSTM to have the efficiency on the test set above 90% for chosen gammas. Such efficiency for chosen gammas is sufficient to our goal, which is to study the relations between the system and control pulses for relatively small disturbances.

B. Robustness of the approximation

The principal aim of this work is to obtain a highly efficient approximation which exhibits known features of the model. In this section, we show the results of an experiment, which allows checking if $\text{ANN}()$ function behaves similarly when the change is introduced to control $h_x(t)$ or control $h_z(t)$ in the same time slot. We perform local disturbances on a set of random NCP, and we check what is the deviation of the new nnDCP from the original DCP. We expect that deviations corresponding to the disturbances on different control fields, but in the same time slot, will be similar.

Let us suppose that we have a trained LSTM. The procedure of checking its sensitivity on variations of $h_j(t)$, for $j \in \{x, z\}$ and t in the i -th time slot, is as follows.

Step 1 Select a NCP vector from the testing set and generate the corresponding nnDCP.

Step 2 If the fidelity between target operator and operator resulting from nnDCP is lower than 90% return to **Step 1**.

Step 3 Select $i \in \{0, \dots, n-1\}$, $j \in \{x, z\}$, change (i, j) coordinate of NCP by fixed ε

- if $\text{NCP}_{i,j} < 1 - \varepsilon$, then $\text{NCP}_{i,j} + \varepsilon$,
- if $\text{NCP}_{i,j} > 1 - \varepsilon$, then $\text{NCP}_{i,j} - \varepsilon$,

and calculate new collection of nnDCP vectors with elements $\text{nnDCP}^{i,j}$, denoting that the element was obtained by perturbing j -th component at the i -th time slot.

Step 4 If the fidelity between target operator and operator resulting from $\text{nnDCP}^{i,j}$ is lower than 90% return to **Step 3**.

Step 5 Calculate norm l_2 (Euclidean norm) of difference between nnDCP and $\text{nnDCP}^{i,j}$.

Because of outlier results of the network, there are additional conditions on generated DCP in the above algorithm. Applying the above algorithm for each NCP from the testing set we can obtain a sample of variations. Next, we can analyse empirical distributions of these variations.

As an example of using the above method we consider the following example. Let us suppose that the drift operator is of the form

$$H_\gamma = \gamma \sigma_y \otimes \mathbf{1}. \quad (12)$$

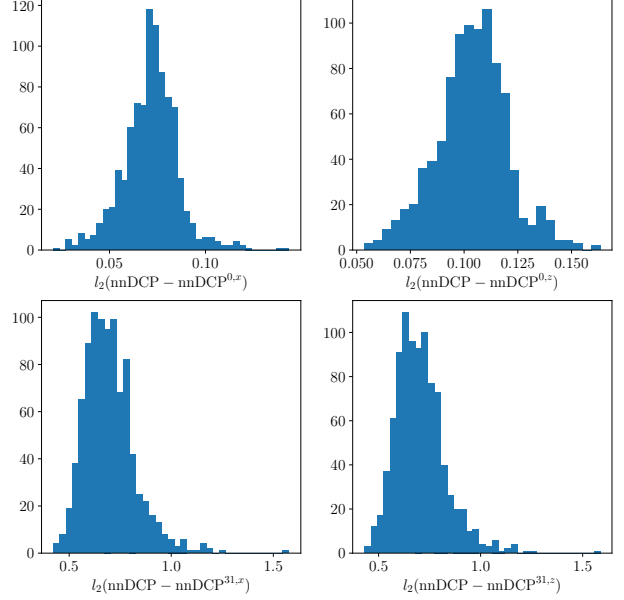


FIG. 1. Exemplary histograms performing variation of ANN approximation. Histograms are generated from disturbances on set of 1000 NCP corresponding to random matrices, for fixed system $H_\gamma = \gamma \sigma_y \otimes \mathbf{1}$.

Then, for $\varepsilon = 0.1$ and $\gamma = 0.2$, the exemplary variation histograms are presented in Fig. 1. Thanks to trained network we are able to analyse the impact of small changes of the input on the output (**Step 5**).

One can consider the median of the distribution of variations as the quantitative measure of the influence of the changes in the input signal on the resulting DCP. To check if medians of distributions of changes are similar, we perform Kruskal–Wallis statistical test for each pair of the changed coordinates (see Fig. 2(a)). Results presented in Fig 2(a) shows that most of the distributions received are statistically different regarding the median, *i.e.* most of the p -values is less than 0.05. The values on the main diagonals, where we compared disturbances on the same controls in the same time slots, are equal to 1. This observation confirms that the test behaves appropriately in this case. On the other hand, one can observe that for time slots $10 \leq i \leq 30$ Kruskal–Wallis test for distributions obtained for $\text{NCP}_{i+1,x} \pm \varepsilon$ and $\text{NCP}_{i,z} \pm \varepsilon$ gives p -values greater than 0.05. Thus, the disturbances introduced in this time slots on h_x and h_z coordinates of NCP results in similar variations of the resulting DCP. The situation is different for time slots $i \leq 10$, where one can see that the variation in DCP signal depends on which coordinate of the NCP signal is disturbed.

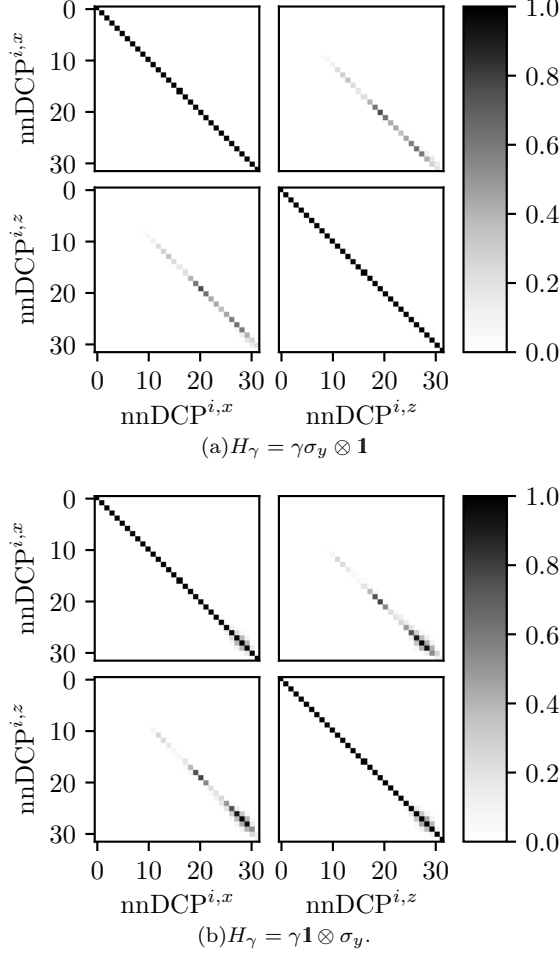


FIG. 2. Plots of p -values of Kruskal-Wallis test for tested drift Hamiltonians. Each element (l, k) of above matrix plots represents a p -value of the test between empirical distributions of changes implied by disturbances on l -th time slot and k -th time slot. The horizontal axis of the left column and the vertical axis of top row plots correspond to disturbances on σ_x control, while horizontal axis of the right column and the vertical axis of the bottom plots correspond to disturbances on σ_z control.

The similar effect can be observed if the drift Hamiltonian acts on the second qubit only. In this case we can consider experiment where the drift Hamiltonian is of the form

$$H_\gamma = \gamma \mathbf{1} \otimes \sigma_y, \quad (13)$$

with $\varepsilon = 0.1$ and $\gamma = 0.2$.

The results of Kruskal-Wallis test for this situation are presented in Fig. 2(b). One can see that our approach suggests that there are similarities in distributions of variations implied by disturbances

on different controls and near time slots. This suggests that local disturbances in control signals have a similar effect in the case of drift on the target system and drift on the auxiliary system.

Moreover, one can see that the constructed approximation exhibits symmetry of the model. This effect can be observed by analysing the disturbances of h_x and h_z controls in the same time slot. From the performed experiments one can see they give similar variations quantified by the distribution of DCP changes.

One should note that on plots in Fig. 2, where we compare variations of $\text{nnDCP}^{i,x}$ and $\text{nnDCP}^{i,z}$, p -values greater than 0.05 are focused along the diagonal. This symmetry is not perfect, but one should note that training data are generated from random unitary matrices. Moreover, as we do not impose any restrictions on the training set to ensure the uniqueness of the correction scheme.

IV. CONCLUDING REMARKS

The primary objective of the presented work is to use artificial neural networks for the purpose of approximating the structure of quantum systems. We propose to use a bidirectional LSTM neural network. We argue that this type of artificial neural network is suitable to capture time-dependences present in quantum control pulses. We have developed a method of reconstructing the relation between control pulses in idealised case and control pulses required to implement quantum computation in the presence of undesirable dynamics. We argue that the proposed method can be useful in studying the relation between the normal control pulses and the de-noising control pulses, rather than efficiently generating de-noising control pulses.

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