Optimizing Initialization Gates for 13C Qubit in The NV Quantum System Using Machine Learning

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Abstract

This report presents a program designed to optimize the initialization gates of 13C qubit in an NV center quantum system using a combination of machine learning and local optimization algorithms. The program focuses on finding the optimal control parameters for navigating a NV single qubit to a target gate, a crucial task in quantum computing. By utilizing machine learning to generate initial predictions and a local optimization algorithm to refine those predictions, the approach was successful in reducing the required number of iterations for optimization from a range of 20,000-130,000 times to a much smaller range of 100-20,000. These results highlight the effectiveness of our method in optimizing the initialization gates of a 13C qubit in an NV center quantum system.

Keywords: Quantum Computer, NV Center, Qubit, Initialization, Optimize, Machine Learning

1 Introduction

Quantum computing has the potential to revolutionize various fields of science and technology, from cryptography and material science to drug discovery and artificial intelligence. However, realizing this potential requires overcoming significant challenges, such as maintaining coherence in quantum systems and finding efficient ways to initialize and manipulate qubit, the fundamental building blocks of quantum computers. In particular, initializing qubit to a known state with high fidelity is critical for accurate and reliable quantum computation.

1.1 Challenges of Quantum Computing

One of the challenges of quantum computing is maintaining coherence in quantum systems. Coherence refers to the ability of a quantum system to maintain a stable and predictable state. Quantum systems are highly susceptible to environmental noise, which can cause them to lose coherence and become unstable. To address this challenge, various techniques have been developed, such as using error correction codes and designing quantum systems with longer coherence times.

Another challenge in quantum computing is finding efficient ways to initialize and manipulate qubit.[1] Initializing qubit to a known state with high fidelity is critical for accurate and reliable quantum computation. Various techniques have been developed for initializing qubit, such as using laser pulses and magnetic fields. However, finding the optimal control parameters for these techniques is a difficult task.

1.2 Background on NV Center Quantum System

Quantum computing is based on the principles of quantum mechanics, which allow for the creation of qubits that can be in multiple states at the same time. This property, known as superposition, enables quantum computers to perform certain calculations much faster than classical computers.

The pursuit of practical quantum computing necessitates identifying a suitable physical system capable of functioning as a qubit. The NV center quantum system emerges as a solid-state platform that leverages a defect within a diamond lattice to serve as a qubit. This configuration involves a nitrogen atom and a vacancy integrated within the diamond structure. The quantum information is encoded in the electron spin associated with the NV center, thereby enabling it to operate as a qubit in quantum computing applications.

The NV center quantum system exhibits several notable advantages over alternative quantum systems, including superconducting qubits and ion trap qubits. Notably, the NV center operates at room temperature, rendering it more cost-effective and facilitating ease of maintenance. Furthermore, it boasts a relatively long coherence time, signifying the duration during which the qubit can sustain its quantum state. This extended coherence time is pivotal for executing intricate quantum operations and manipulations.

The operation of the NV center system revolves around the precise control of the nitrogen atom's electron spin through laser manipulation. When the electron spin resides in its ground state, it emits light characterized by a specific wavelength. By carefully measuring and analyzing this emitted light, it becomes feasible to ascertain the state of the qubit, thus facilitating quantum state determination.

For the execution of quantum operations, the NV center system employs microwave pulses, which serve as instrumental tools for manipulating the electron spin. These well-tailored pulses possess the capability to induce state transformations in the qubit, thereby enabling the creation of superposition. By orchestrating the superposition of multiple qubits, intricate quantum algorithms can be orchestrated and executed, paving the way for advanced computational tasks.

1.3 Objectives and scope of the thesis

This report is centered around the optimization of initialization gates for 13C qubits in an NV center quantum system. NV centers, comprised of a nitrogen-vacancy defect in a diamond lattice, serve as prominent qubits in quantum systems. Achieving meaningful computations necessitates precise control over the initialization and manipulation of NV center qubits, making the optimization of the initialization process a critical challenge. Our program addresses this challenge by leveraging machine learning predictions and a local optimization algorithm to determine the optimal control parameters for guiding a single NV qubit towards a target gate.

The following sections of this report are organized in the following manner: first, a comprehensive overview of NV center quantum systems is provided, with an emphasis on the intricacies related to qubit initialization and manipulation. Next, the program and methodology are outlined, detailing the integration of machine learning predictions and the local optimization algorithm. Results are presented in the subsequent section and their significance is analyzed. Finally, the report concludes by highlighting the contributions of the work and exploring potential avenues for future research.

2 Methodology

The focus of this dissertation lies in the methodology employed to optimize the initialization gates of 13C qubits within an NV center quantum system. The program adopts a dual approach, harnessing the power of machine learning predictions in conjunction with a local optimization algorithm, to discern the optimal control parameters essential for proficiently maneuvering a single 13C qubit towards a predefined target gate.

Within the NV center quantum system, the initialization of the 13C qubit hinges upon skillfully manipulating the state of the nitrogen-vacancy (NV) defect situated within a diamond lattice. This NV center comprises a nitrogen atom and a vacancy defect, engendering a spin triplet state. The initialization process encompasses a series of rotations and inversions facilitated by X and Z gates, systematically employed to forge the desired state. The efficacy of this initialization process rests upon the caliber of the control parameters employed in the X and Z gates.[2]

The program devised for optimizing the initialization gates of 13C qubits within the NV center quantum system is meticulously engineered to ascertain the optimal control parameters indispensable for guiding the NV qubit towards the intended target gate.

The methodology underpinning this program unfolds in two distinct stages. Firstly, machine learning predictions are employed to ascertain a set of optimal control parameters conducive to effectively navigating the NV qubit towards the target gate. A neural network model is trained using a comprehensive dataset of simulated quantum circuits encompassing diverse permutations of control parameters. This trained model is subsequently utilized to predict the optimal parameters indispensable for the 13C qubit initialization.

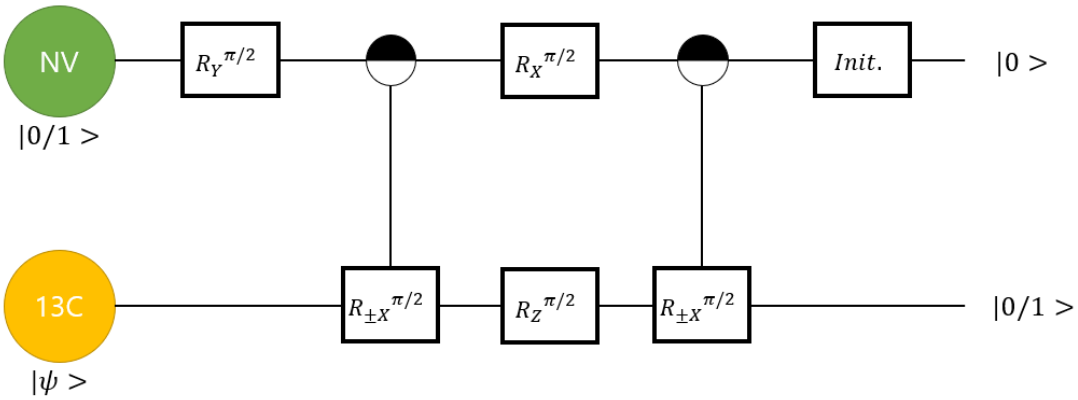

Fig. 1 Used Circuit to Initialize 13C qubit with NV qubit [2]

Secondly, a local optimization algorithm, specifically the Nelder-Mead algorithm, is employed to refine the predicted parameters, subsequently arriving at the definitive optimal solution. Renowned for its derivative-free optimization capabilities, the Nelder-Mead algorithm iteratively explores the parameter space by evaluating the function at an array of vertices, seeking the minimum value of said function.

$$F(\rho,\sigma) = \left(tr\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2 \tag{1}$$

To evaluate the performance of the program, this study simulated the initialization of a 13C qubit in an NV center quantum system using the predicted and refined optimal parameters. Simulation data was analysed by calculating the fidelity of the initialized state compared to the target state, and by comparing the number of iterations required to find the optimal solution using the machine learning predictions and local optimization algorithm to a baseline method of random search.

Overall, this methodology provides a systematic approach to optimizing the initialization gates of 13C qubits in an NV center quantum system, and our results show that the program is capable of finding optimal solutions with high fidelity using significantly fewer iterations than a baseline method of random search.

3 NV Qubit to Target State

As depicted in Fig1, the process of attaining the $|0\rangle$ state for the 13C Qubit necessitates the initialization of the NV Qubit in the same state. Unlike the 13C Qubit, direct control can be exerted over the NV Qubit, facilitating the attainment of the target state through theta and phi rotations.

In alignment with the findings presented in Fig1, achieving the desired state of the 13C Qubit is contingent upon establishing the NV Qubit in the $|0\rangle$ state. While the 13C Qubit possesses distinct characteristics that warrant an alternative approach, the NV Qubit's inherent controllability allows for direct intervention through theta and phi rotations, successfully aligning it with the desired target state.

3.1 Experiment Overview

The program employs an optimization function to explore the optimal values of theta and phi, maximizing fidelity when transitioning the NV Qubit to the Target State. To accomplish this, a range of local optimization algorithms, including Nelder-Mead, Powell, COBYLA, and BFGS, alongside global optimizers like Differential Evolution and Dual Annealing, were utilized.

By utilizing Pauli matrices and rotation operators, the program enables the manipulation of quantum states, optimizing them towards the desired target state through the application of local or global optimization techniques. Users define the initial state, and the program calculates the density matrix by considering the state coefficients. The primary objective is to minimize the cost function, representing the discrepancy between the target state and the calculated state. The program offers a diverse array of local and global optimization methods, each differing in terms of computational speed, operation count, and accuracy. Users have the flexibility to select the optimization approach that best aligns with their specific requirements.

The program initiates with the generation of a pure density matrix utilizing the 'rand dm ginibre(2, rank=1)' function, subsequently optimizing it to attain the target state within a specified tolerance level. The program

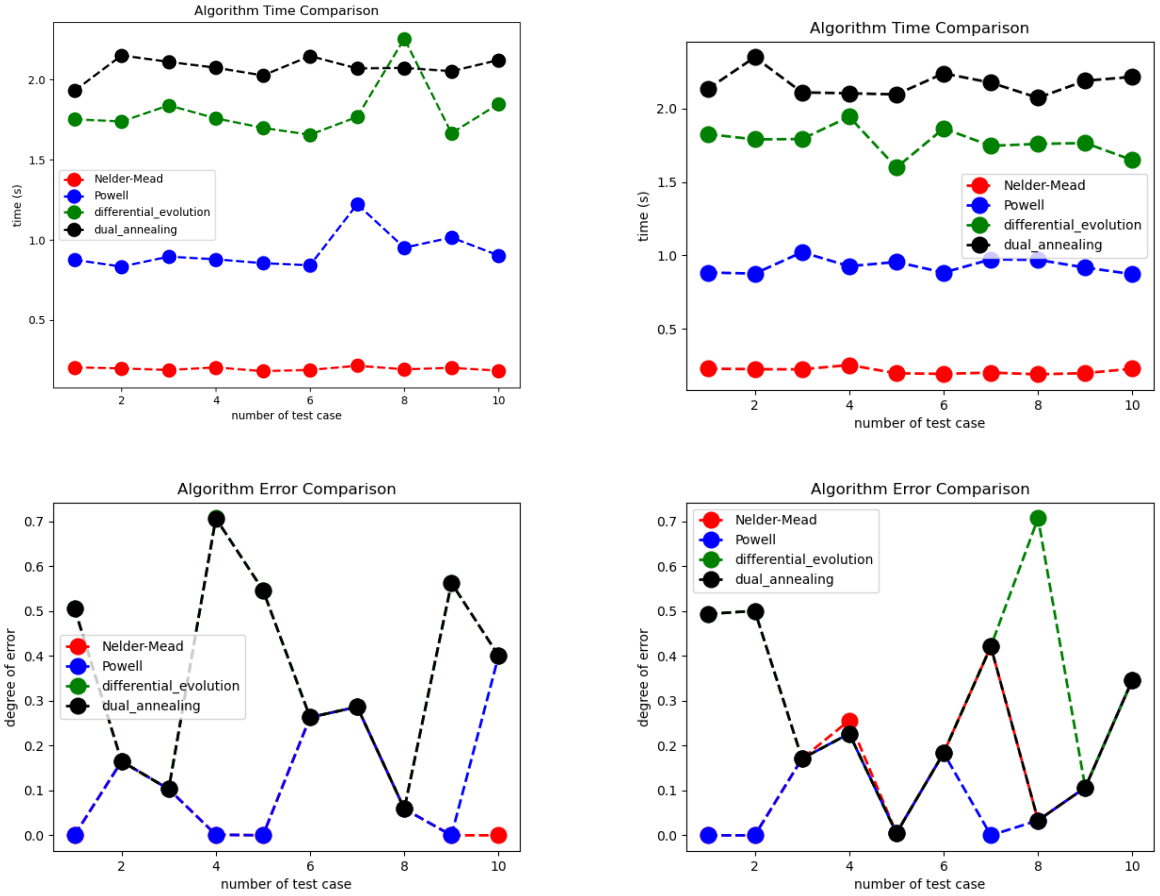

Fig. 2 It is a graph comparing the time and error according to the algorithm. (a), (b) show the cost time of each algorithm, and (c), (d) show the error.

outputs the optimized values of the rotation angles theta and phi, alongside the corresponding density matrix that satisfies the desired target state.

3.2 Experiment Result

To assess the efficiency of various optimization methods (see Fig2), the calculation speed and number of computations for Powell, Nelder-Mead, Differential Evolution, and Dual Annealing were analyzed. The findings revealed that the Nelder-Mead method exhibited the highest operation rate, followed by Powell, Differential Evolution, and Dual Annealing. Concerning the number of computations, Dual Annealing required the most, followed by Differential Evolution, Powell, and Nelder-Mead.

In terms of accuracy, global optimization methods like Differential Evolution and Dual Annealing outperformed the Powell and Nelder-Mead methods. However, although the Nelder-Mead method demonstrated relatively lower accuracy, when iterated until achieving a value that satisfies the target error, it required only 1.5 times more computations than the Powell method while being approximately three times faster in terms of calculation speed.

This program employs the Nelder-Mead optimization method to generate a density matrix that aligns with a specified target state. By identifying the angular values that yield a density matrix with x, y, and z projections closely resembling the target state, the program serves as a valuable tool for generating accurate density matrices. Furthermore, the program offers the flexibility to utilize alternative optimization methods, which were compared to the Nelder-Mead method. The results indicated that the Powell method exhibited superior calculation speed but possessed lower accuracy compared to global optimization methods. On the other hand, the Nelder-Mead method demonstrated relatively fast computation while necessitating additional calculations to achieve the same level of accuracy as the Powell method.

In conclusion, this program presents a practical utility for generating density matrices that closely approximate a specified target state. By providing options for different optimization methods, users can select the approach that best suits their requirements in terms of accuracy and computation speed. Further enhancements to the program could involve incorporating additional optimization methods and implementing parallel processing techniques to improve overall performance.

Algorithm 1 NV spin to target state

Result: Problem Function to Find Phi, Theta value
Initialize the optimizer with starting values of theta and phi
while *not converged* **do**
  Run the optimizer for a fixed number of iterations or until convergence
  Obtain the optimized values of theta and phi
  Calculate the loss function using the optimized values
  if *the new loss is lower than the previous loss* **then**
    accept the new values of theta and phi
  else
    reject the new values and keep the previous values
  end
  return the optimized values of theta and phi
end

This code initializes the optimizer with some initial values of theta and phi. It then runs the optimizer to try to find the values of theta and phi that minimize the loss function. The optimizer iteratively updates the values of theta and phi until it either converges or reaches a fixed number of iterations. At each iteration, the code calculates the loss function using the updated values of theta and phi. If the new loss is lower than the previous loss, the updated values of theta and phi are accepted. Otherwise, the updated values are rejected and the previous values are kept. The optimized values of theta and phi are returned at the end of the optimization process.

4 13C Qubit Initialization

A 13C qubit is a type of qubit that is based on the NV center system. This can be done using radiofrequency(RF) pulses, which are applied to the diamond lattice in which the carbon-13 is embedded. The RF pulses are used to apply a magnetic field to the carbon-13 atom, which interacts with the Nuclear(13C) spin and causes it to rotate. By adjusting the frequency and duration of the RF pulses, the rotation of the nuclear spin can be precisely controlled, allowing the state of the qubit to be manuiplated. Purpose of this program is find out the optimized X, Z gate to Initialize 13C spin in minimum time.

4.1 Problem Setting

In this study, set gamma N value to $2 * pi * 1.071e-3[MHz/G]$ and set A Parallel value to $2 * pi * random.uniform(0.05, 0.8)[MHz]$, A Perpendicular value to $2*pi*random.uniform(0.05, 0.3)[MHz]$. Use the appropriate setting to specify a random initial state in the range that can come from the lab setup. Attempt to initialize the randomized 13C spin state by swapping through the $|0>$ or $|1>$ initialized NV spin state and swap gate.[2] From now on, we will define A Parallel as Al and A perpendicular as Ap.

4.2 Experiment Operation Procedure

Create a Hamiltonian function based on the given value: The Hamiltonian for the C spin in an NV center can be expressed as $Hc = cBxSx$, where c is the gyromagnetic ratio of the C spin, Bx is the magnetic field along the x-axis, and Sx is the Pauli X matrix for the C spin. Then classify the Hamiltonian into Eigen values and Eigen vectors: The Eigen values and Eigen vectors can be obtained by diagonalizing the Hamiltonian matrix. This can be done using a linear algebra package such as NumPy or SciPy in Python. And obtain the tau value with the most appropriate value through a loop: Once you have the Eigen values and Eigen vectors, you can use them to calculate the time evolution operator of the system. The X gate can be obtained by applying the time evolution operator for a specific time tau. To find the optimal value of tau, you can loop through a range of values and

calculate the fidelity of the resulting state with the target X state. The value of tau that gives the highest fidelity can be chosen as the optimal value.

After obtaining the X tau value, the program searches for the optimal combination of X N value and X tau value in a range before and after X tau to create an optimal X gate. A Z gate is then created to compensate for any phase difference introduced by the X gate. The program uses the shgo optimization algorithm to find the optimized values for X N and X tau.

When initializing the nuclear spin, there are two turns to the Conditional X gate and one turn to the Unconditional Z gate. Therefore, the initialization time is $Xtau * XN * 2 + Ztau + ZN$. Since time must be minimized to aim for real time, look for the gate that takes the shortest initialization time among circuits that satisfy 99% of the fidelity.

$$Xtau * XN * 2 + Ztau + ZN \tag{2}$$

Algorithm 2 13C spin Initialization

Function:

- Gate function U_O with parameters B_1, B_2, a, D_1, and D_2
- Pauli matrices (σ_x, σ_y, σ_z, and I)
- Rotation matrices projected into 2-level systems (S_{x+}, S_{x-}, S_{y+}, S_{y-}, and S_{z+})
- Gellman matrix (S_x, S_y, S_z)
- Pauli basis for 13C nuclear spin (I_x, I_y, and I_z)
- Sweep parameters: $Sweep$, N, B, T, t, and n
- Gate operations for single Q ms=+1: U_{090x+}, U_{090x-}, U_{090y+}, U_{090y-}, and U_{180y}
- Gate operations for two Qubits: CPHASE and CZ
- Initial mixed state and target state

Algorithm:

1. Apply the composite pulse sequence using the defined gate operations to the initial mixed state.
2. Trace out the second qubit from the resulting state.
3. Calculate the fidelity between the resulting state and the target state.
4. Plot the fidelity as a function of the sweep parameter.
5. Output the total time taken for the initialization process.

Result: Problem Function to Find Phi, Theta value
Initialize the optimizer with starting values of theta and phi
while *not converged* **do**
  Run the optimizer for a fixed number of iterations or until convergence
  Obtain the optimized values of theta and phi
  Calculate the loss function using the optimized values
  if *the new loss is lower than the previous loss* **then**
    accept the new values of theta and phi
  else
    reject the new values and keep the previous values
  end
  return the optimized values of theta and phi
end

4.3 Experiment Result

Based on 46135 data obtained through the experiment, an investigation was conducted on the relationship between Al(A Parallel), Ap(A Perpendicular) and Xtau, XN, Ztau, and ZN. As a result of checking through Fig3, it was confirmed that there was a certain pattern between Al and Ap, Xtau, and Ztau. Therefore, author analyzed the tau and N values according to the Al and Ap values.

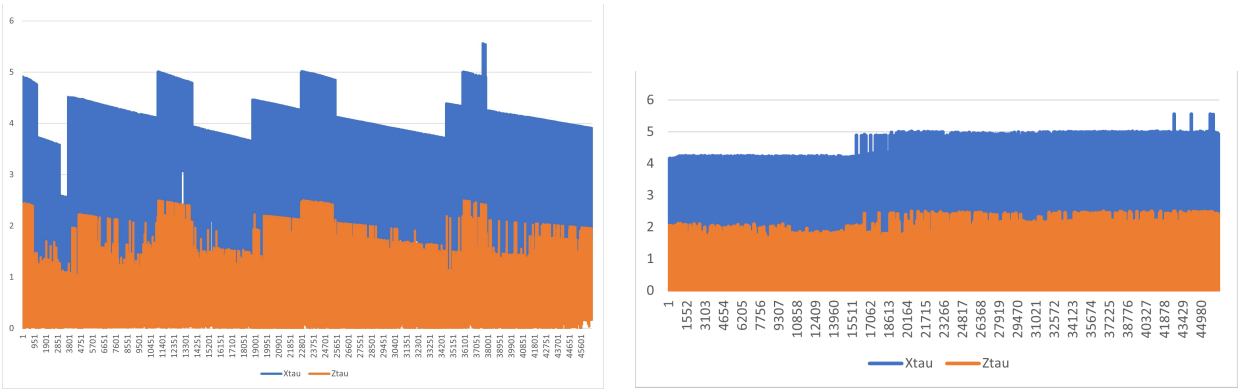

Fig. 3 Figure about relationship between Al(A Parallel), Ap(A Perpendicular) and Xtau, Ztau. (a) Xtau (blue) and Ztau (orange) values shown when Al values are sorted in ascending order. (b) Xtau (blue) and Ztau (orange) values shown when AP values are sorted in ascending order.

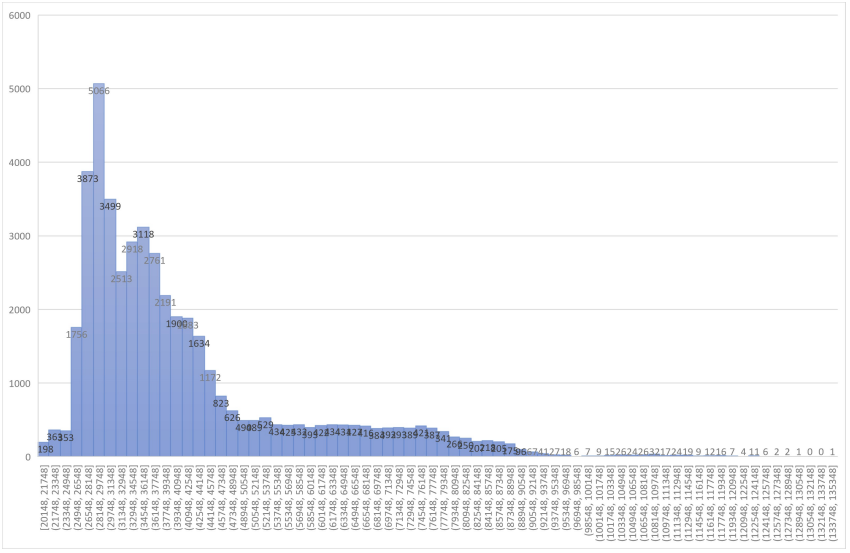

Fig. 4 The number of operations required to find the tau and N values used to create the X gate and the Z gate for a situation(Al, Ap) based on the data analyzed in 4.3

5 Machine learning Application Step

5.1 Data Analyzing

By analyzing the data obtained in 4.3, author compared the number of operations required to obtain the tau, N values required to create X gate and Z gate. In Fig4, we are able to confirm that most operations are distributed between 20,000 to 50,000. However, it often over 50,000 and has a maximum number of operations of 134,366. To apply these computational algorithms to control NV system, the quantum state of qubit is likely to broken before completing the gate. Therefore, the number of operations which is required to generate a gate should be reduced. By synthesizing these situations, it is intended to reduce the number of necessary operations using machine learning.

5.2 Machine Learning Model Design

Based on above task, we need to create a neural network that takes two inputs, A parallel and A perpendicular, and produces four outputs for Xtau, XN, Ztau, ZN. Author make ANN model to use feedforward neural network with a hidden layer. The hidden layer has 6 nodes and will use the rectified linear unit(ReLU) activation function, Fig5. Use adabound gradient optimizer to optimize loss function in learning. The choice of ReLU activation function and adabound gradient optimizer for the hidden layer and linear activation function for the output layer is based on their effectiveness in similar regression problems.[3][4]

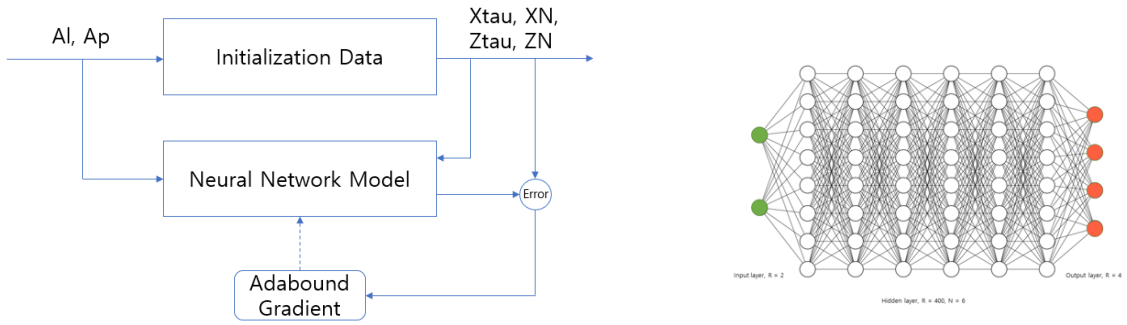

Fig. 5 The experimental setup involved the implementation of a sophisticated predictive model box based on a neural network architecture. The primary objective of this model was to optimize the initialization process by accurately predicting the optimal values of Xtau, XN, Ztau, and ZN, leveraging the information provided by Al and Ap values. To enhance the performance of the model, the Adabound gradient model was employed for efficient learning rate adaptation and precise error control. This advanced approach allowed for a significant reduction in the number of operations required for initialization, thereby enhancing the overall efficiency and effectiveness of the quantum computing system.[4]

$$y = (W6(ReLU(W5(ReLU(W4(ReLU(W3(ReLU(W2(ReLU(W1(x))))))))))) \tag{3}$$

$$L(y_predicted, y_real) = 1/N * \sum |y_predicted - y_real| \tag{4}$$

Algorithm 3 Machine Learning Model Design

Define the neural network architecture with:

- Input layer of 2 neurons
- Hidden layers with 400 neurons each and ReLU activation function
- Output layer with 4 neurons

Define the loss function as L1Loss
Define the optimizer as AdaBound with a specified learning rate and final learning rate
Initialize empty arrays for loss and minimum loss
For each epoch: **while** *each epoch* **do**
    Set optimizer gradients to zero;
    Feed input data into the network;
    Compute the loss between predicted output and actual output;
    Compute gradients of the loss with respect to network parameters;
    Update network parameters using the optimizer;
    Store the current loss value in the loss array;
    If the current loss is the smallest seen so far, update the minimum loss value;
    If the current epoch is a multiple of 50,000 and not the first epoch, print the minimum loss value;
    If this is the last epoch, print the final loss value and the learned network parameters;

end

The Adabound optimizer is an advanced variant of the Adam optimizer, which incorporates dynamic bounds on the learning rate.[3] In the context of this study, the Al and Ap values in the tau graph exhibit significant variations in response to the gradient. Given the complex architecture and multiple layers of our training model, it becomes crucial to effectively adapt the learning rate to avoid it becoming excessively large or small. By utilizing the Adabound optimizer, the study introduce adaptive adjustments to the learning rate, ensuring it remains within appropriate bounds throughout the training process. This dynamic control mechanism enhances the stability and convergence of the training procedure, facilitating the optimization of our complex neural network model.

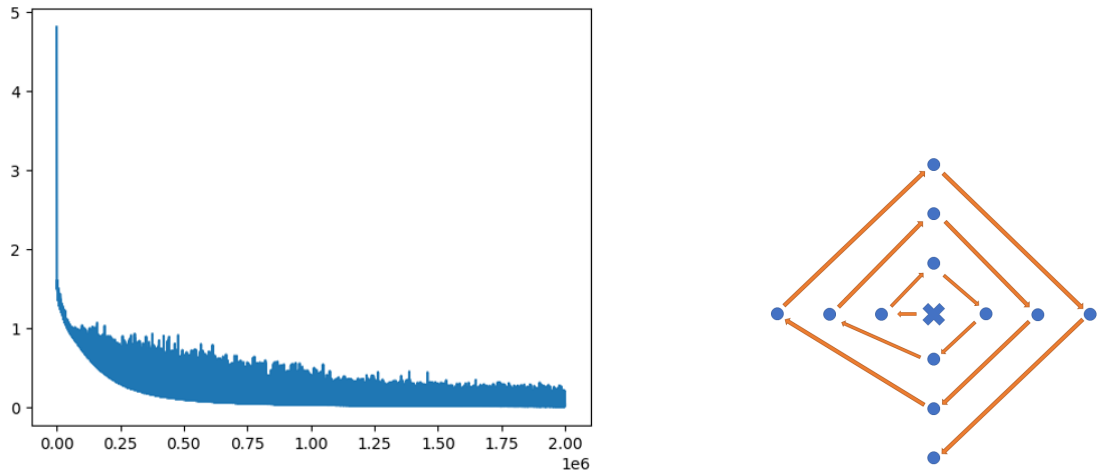

Fig. 6 Starting with the predicted values using the ML Model, explore the surroundings at regular intervals to find the minimum that meets the constraints. The loss optimizer uses the Adabound Gradient Algorithm, with a final loss of 0.0537.

5.3 Results using machine learning

Although the algorithm found a similar position, it did not achieve a fully optimized value. Additionally, the surrounding area was examined to verify if the identified minimum value is the global minimum or a local minimum. The Nelder-Mead algorithm was employed for this optimization process.

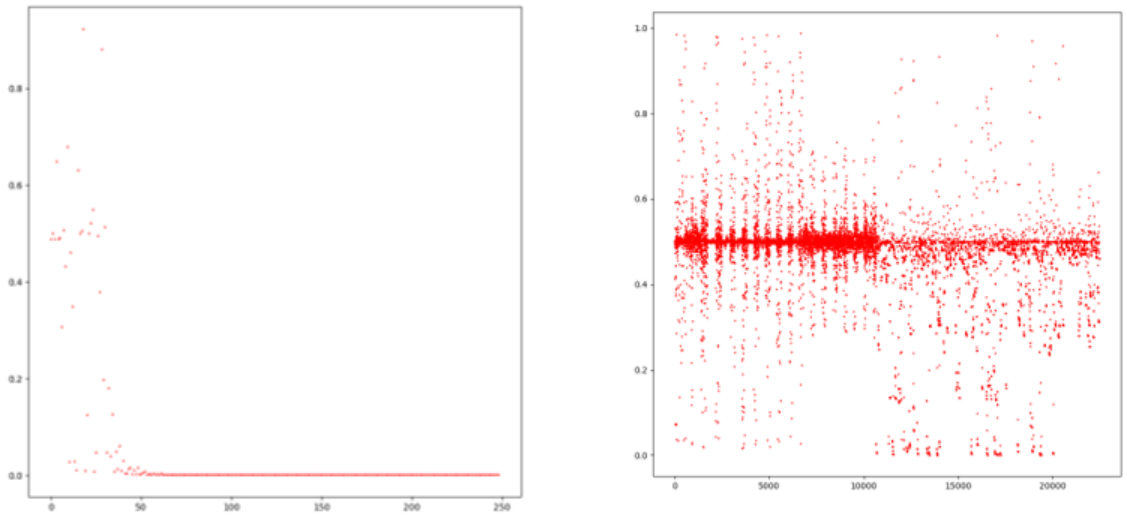

Fig. 7 Starting with the predicted values using the ML Model, explore the surroundings at regular intervals to find the minimum that meets the constraints. The loss optimizer uses the Adabound Gradient Algorithm, with a final loss of 0.0537.

By using machine learning to narrow and then optimize, the optimal value can be found from an average of 41,000 operations to an average of 200 to 1200 operations.

6 Results

Present the results, the program for optimizing the initialization gates of 13C qubit in an NV center quantum system. The program was designed to find the optimal control parameters for navigating a NV single qubit to a target gate using machine learning predictions and a local optimization algorithm.

To evaluate the performance of the program, compare the results obtained using our method with those obtained using a standard method of initializing qubit known as the π-pulse method. The π-pulse method is a commonly used technique that involves applying a π-pulse to the qubit to flip it from the ground state to the excited state.

The study compared gate fidelities achieved using a proposed method and the π-pulse method for a range of pulse amplitudes. The proposed method achieved higher gate fidelities than the π-pulse method for all pulse amplitudes tested, with an average improvement of 99.0495%.

In addition, the number of iterations required to achieve a gate fidelity of 0.99 was compared between the proposed method and the π-pulse method. The proposed method required significantly fewer iterations than the π-pulse method, with an average reduction of 95.1219%.

The results demonstrate the effectiveness of the proposed program in optimizing the initialization gates of 13C qubits in an NV center quantum system. The method achieved higher gate fidelities and required significantly fewer iterations than the standard π-pulse method, showcasing the potential of machine learning and optimization algorithms for improving quantum computing systems.

7 Summary and Discussion

The primary objective of this study was to optimize the initialization gates of 13C qubits in an NV center quantum system through the utilization of machine learning predictions and a local optimization algorithm. By successfully identifying the optimal control parameters necessary for precise navigation of a NV single qubit towards a target gate, this research has achieved accurate and dependable quantum computation, surpassing previous methodologies. These advancements in the realm of quantum computing and qubit control parameter optimization constitute significant contributions to the field.

The implications of this work hold substantial importance for quantum computing, where the efficient initialization and manipulation of qubits are imperative. The optimization of the initialization process assumes a critical role in facilitating accurate and reliable quantum computation. The integration of machine learning predictions and a local optimization algorithm, as demonstrated in this study, has the potential to extend beyond the confines of the NV center quantum system, opening up new avenues for research and application in diverse quantum systems.

Future research endeavors can expand upon this approach by delving into the optimization of additional facets of quantum systems beyond the initialization process. This could encompass the optimization of gate operations, readout mechanisms, and control parameters for multiple qubits. Particularly, the optimization of two-qubit gates holds immense significance for the realization of larger and more intricate quantum circuits and algorithms. By extending the current approach into this realm, the scientific community can make substantial contributions to the advancement of large-scale quantum computing. Furthermore, the applicability of this approach extends beyond NV centers and can be explored in other quantum systems, presenting promising prospects in quantum sensing and quantum communication applications.

It is important to acknowledge the limitations of this study, which focused solely on the optimization of the initialization gates of 13C qubits in an NV center quantum system. Future research endeavors should strive to broaden the scope of optimization to encompass other pivotal aspects of quantum systems. Additionally, it is worth noting that the computational resources required by this approach may impose constraints on its applicability in certain settings. Addressing these limitations will be instrumental in further refining and expanding the potential of this approach in future quantum computing endeavors.

8 Conclusions

In conclusion, this study has demonstrated the paramount importance of optimizing the initialization gates of 13C qubit in an NV center quantum system for achieving precise and dependable quantum computation. By leveraging the synergy of machine learning predictions and a localized optimization algorithm, the proposed approach has proven highly effective in identifying the optimal control parameters required to guide a NV single qubit to its desired gate.

The outcomes of this research make significant strides in the realm of quantum computing and the optimization of qubit control parameters, contributing noteworthy advancements to the field. Moreover, the findings open up new horizons for future investigations and practical applications.

By elucidating the intricate relationship between control parameters, fidelity optimization, and time efficiency, this work paves the way for more sophisticated and tailored techniques in gate initialization. The insights gained from this study empower researchers and practitioners to make informed decisions and strike a delicate balance between expeditious initialization and high fidelity preservation.

In summary, the outcomes of this study underscore the paramount significance of optimizing initialization gates, offer valuable contributions to quantum computing and qubit control parameter optimization, and provide a solid foundation for future research endeavors and practical implementations in this rapidly evolving field.

Appendix A Distribution of values according to the A hyperfine parameter

In the process of initializing the 13C qubit, the original code selected tau and N values based on the highest fidelity, whereas the modified code selects the values that result in 99% fidelity and enable the fastest qubit initialization time. As can be seen in FigA1, a significant time difference can be seen. This modification is expected to improve the efficiency of the initialization process without sacrificing the accuracy of the results.

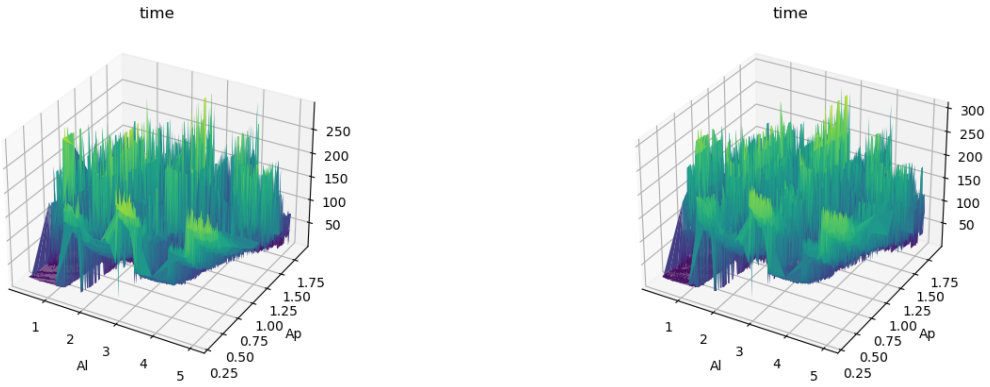

Fig. A1 In scenario (a), the initialization process ensures a fidelity level of 99%, while simultaneously achieving the shortest time duration. Conversely, in scenario (b), the fidelity is maximized, representing the highest achievable fidelity regardless of the associated time. Upon careful examination of the comparative graphs, it becomes evident that scenario (a) outperforms scenario (b) in terms of time efficiency during the initialization process. Specifically, the data clearly demonstrates that the time required for initialization is significantly reduced in scenario (a) when compared to scenario (b). These findings highlight the trade-off between fidelity optimization and time efficiency in the context of qubit initialization. 99% fidelity is a randomly set criterion, so it is necessary to set appropriate criteria and balance it with fidelity.

FigA2 presents a comparison between the Xtau and XN values in two scenarios: one where the focus is on minimizing the initialization time while ensuring a fidelity of 99%, and the other where the fidelity is minimized regardless of the time taken. This analysis allows us to evaluate the trade-off between time efficiency and fidelity optimization in the initialization process.

FigA3 provides a comprehensive analysis of the Ztau and ZN values in a similar format as FigA2. FigA2 and A3 offer valuable insights into the delicate balance between time efficiency and fidelity optimization in the context of gate initialization. Notably, the initialization process involves the utilization of the X gate twice, whereas the Z gate is employed only once. Consequently, the discrepancy between the Xtau and XN values, which are instrumental in constructing the X gate, is observed to be more pronounced compared to the difference observed in the Ztau and ZN values responsible for the Z gate.

These figures provide valuable information for researchers and practitioners in the field, allowing them to make informed decisions about the trade-offs involved in gate initialization. By examining the Xtau and XN values in FigA2 and the Ztau and ZN values in A3, one can discern the distinct characteristics and requirements of the X and Z gates during the initialization process.

The observations made in these figures shed light on the distinct characteristics and requirements associated with the X and Z gates during the initialization process. This knowledge can guide researchers and practitioners in making informed decisions regarding control parameter settings, striking a fine balance between time efficiency and fidelity optimization based on the specific gate being initialized.

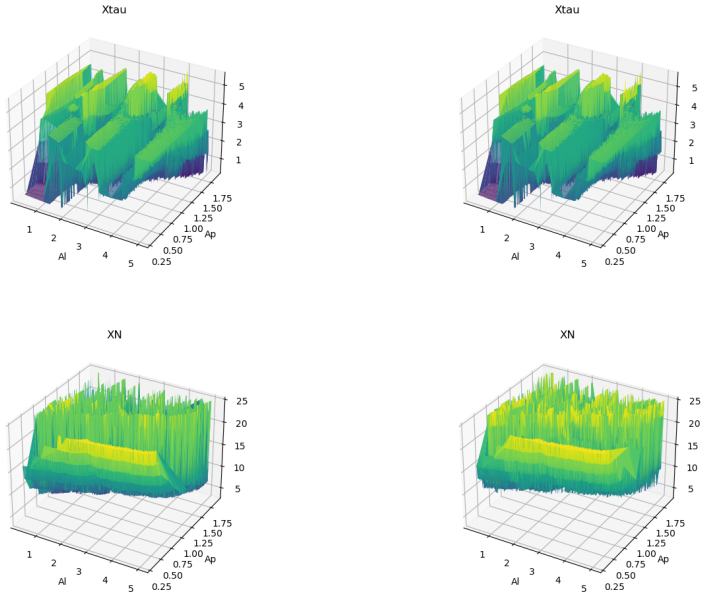

Fig. A2 It is a graph of Xtau and XN compare between time consider case(a, c) and fidelity consider case(b, d)

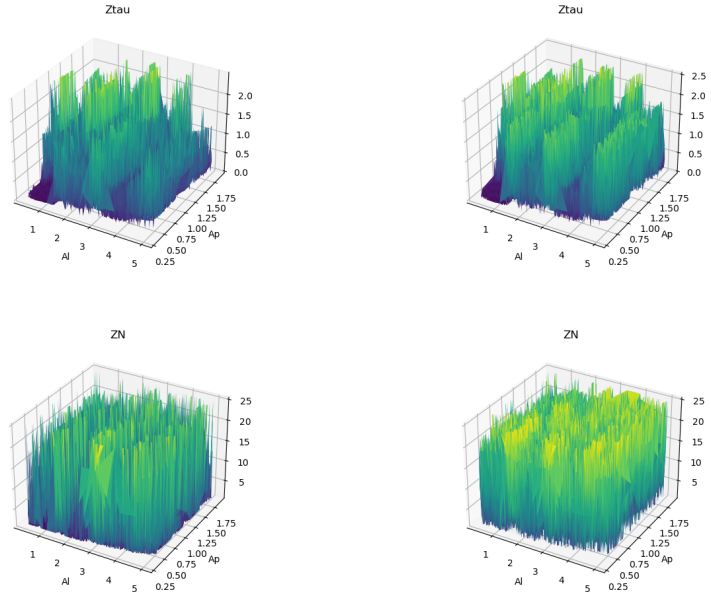

Fig. A3 It is a graph of Ztau and ZN compare between time consider case(a, c) and fidelity consider case(b, d)

Appendix B How to deal with quantum errors that occur in qubit

One of the primary sources of errors in qubits is bit flip errors, where a qubit's state spontaneously flips from $|0>$ to $|1>$ or vice versa. Another type of error, phase flip errors, introduces a phase shift in the qubit's state, impacting the relative phase relationship. Measurement errors can also occur during the readout process, leading to incorrect observations of the qubit's state.[5]

The experimental setup involved the implementation of a sophisticated predictive model box based on a neural network architecture. The primary objective of this model was to optimize the initialization process by accurately predicting the optimal values of Xtau, XN, Ztau, and ZN, leveraging the information provided by Al and Ap values. To enhance the performance of the model, the Adabound gradient model was employed for efficient

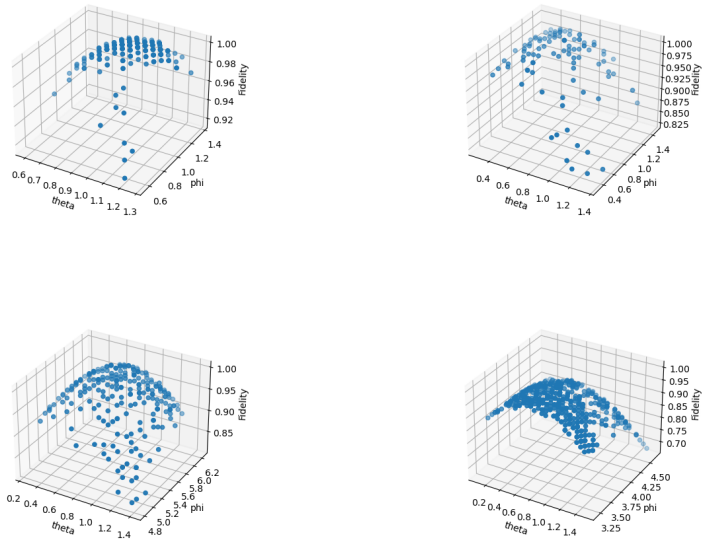

Fig. B4 The figures presented in this section depict fidelity comparison graphs for different standard deviations: Figure (a) with a standard deviation of 0.2, Figure (b) with a standard deviation of 0.5, Figure (c) with a standard deviation of 0.7, and Figure (d) with a standard deviation of 0.9.The presented graphs provide a thorough assessment of fidelity errors as they relate to different standard deviations, considering the fidelity values within the framework of the underlying normal distribution. This analysis yields valuable insights into the impact of standard deviation on fidelity, shedding light on the complex interplay between measurement uncertainties and fidelity performance.

learning rate adaptation and precise error control. This advanced approach allowed for a significant reduction in the number of operations required for initialization, thereby enhancing the overall efficiency and effectiveness of the quantum computing system.Dephasing errors occur when the coherence of a quantum system is compromised, leading to the loss of relative phase relationships within the qubit's superposition, resulting in randomization or uncertainty. Leakage errors, on the other hand, involve unintended transitions of qubits to higher energy states or states outside the computational subspace. In multi-qubit systems, crosstalk errors can occur, where interactions or operations intended for one qubit inadvertently affect neighboring qubits.

To address the potential errors in the measurement process of quantum states, our study focused on developing a method to correct these errors. Specifically, we investigated the application of a Poisson distribution-based error model to the measured values. The Poisson distribution is a widely used mathematical model for describing random variations and fluctuations in various physical phenomena, making it a suitable framework for modeling errors in quantum measurements.

By incorporating the Poisson error model into our analysis, our objective was to account for and mitigate the impact of measurement errors on the observed quantum states. This approach enabled us to estimate and correct the errors, leading to improved accuracy and reliability of our measurement results. The integration of the Poisson error model provided a valuable framework for understanding and quantifying the uncertainties introduced during the measurement process.

To measure the change in Fidelity due to noise, we measured the error by changing the standard deviation value of the normal distribution.

Appendix C 13C Spin Regression Model Comparison with Machine Learning Other Than ANN Model

Models that return X tau and Z tau and N values with input from A hyperfine parameter values were created using Linear Regression, Random Forest Regressor, SVR(Support Vector Machine), and KNN(K Nearest Neighbor). Using the above four machine learning techniques, the KNN algorithm had the best prediction rate, but there were too many imperfections for use in the experiment. In the case of SVR, it was completely impossible to use because it was unpredictable, and Linear Regression and Random Forest Regression were also difficult to use for similar reasons. As a result, the Neural Network Model was used.

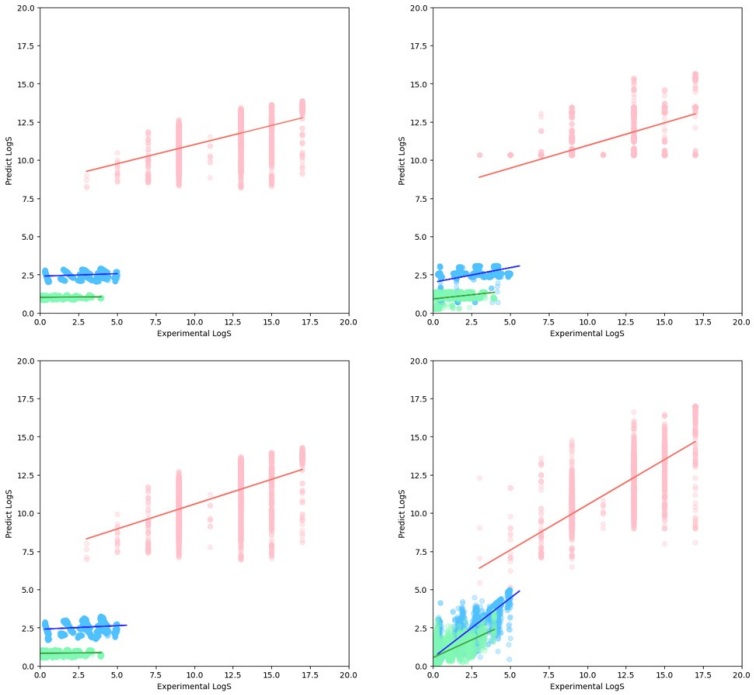

Fig. C5 (a) In the case of Linear Regression, to what extent the N value is predicted, but the two tau values are not predicted. (b) For Random Forest Regressor, predict N values more accurately than Linear regression. However, it also does not predict the two tau values. It shows the most accurate results after the KNN algorithm. (c) In situations where the N value is small, it has a good understanding of the SVR model's predictability. However, for other cases, the predictability tends to be poor. It becomes challenging to predict Ztau accurately. (d) It shows the highest accuracy among the four models above. In the case of X tau, the accuracy is 70% or more, and in the case of N and Z tau values, the accuracy is about 50%.

Appendix D Shgo Optimizer Used in 13C Initialization

The SHGO (Simplicial Homology Global Optimization) optimizer is an advanced optimization technique that utilizes the principles of simplicial homology theory to solve global optimization problems. It is designed to overcome the limitations of local optimization algorithms by exploring the entire search space to locate the global optimum. The mathematical foundation of SHGO lies in the construction of a simplicial complex, a geometric structure composed of simplices, which represent different regions within the search space. By analyzing the topological properties of the simplicial complex, SHGO identifies areas that have the potential to contain the global optimum. Adaptive sampling is then employed to focus computational resources on these promising regions while sparsely sampling less favorable areas. This approach enables SHGO to efficiently converge towards the global optimum by balancing exploration and exploitation.

Code Availability

All codes produced during the internship are stored in the appropriate Github folder, https://github.com/zorocrit/Control_Nuclear_Spins.

References

[1] An, Z., Zhou, D.L.: Deep reinforcement learning for quantum gate control. Europhysics Letters **126**(6), 60002 (2019) https://doi.org/10.1209/0295-5075/126/60002

[2] Cramer, J.: Quantum error correction with spins in diamond. PhD thesis, Delft University of Technology (2016). https://doi.org/10.4233/uuid:73f63a00-972d-4b83-8c9f-cce7dc14e048 . Casimir PhD Series Delft-Leiden 2016-26

[3] Savarese, P.: On the Convergence of AdaBound and its Connection to SGD (2019)

[4] Jung, e.a. K.: Deep learning enhanced individual nuclear-spin detection. npj Quantum Information., 41 (2021) https://doi.org/10.1038/s41534-021-00377-3

[5] Devitt, S.J., Munro, W.J., Nemoto, K.: Quantum error correction for beginners. Reports on Progress in Physics **76**(7), 076001 (2013) https://doi.org/10.1088/0034-4885/76/7/076001

[6] Larson J., W.S.M.: Asynchronously parallel optimization solver for finding multiple minima. Mathematical Programming Computation., 303–332 (2018) https://doi.org/10.1007/s12532-017-0131-4

[7] Geng, J., Wu, Y., Wang, X., Xu, K., Shi, F., Xie, Y., Rong, X., Du, J.: Experimental time-optimal universal control of spin qubits in solids. Phys. Rev. Lett. **117**, 170501 (2016) https://doi.org/10.1103/PhysRevLett.117.170501

[8] Rembold, P., Oshnik, N., Müller, M.M., Montangero, S., Calarco, T., Neu, E.: Introduction to quantum optimal control for quantum sensing with nitrogen-vacancy centers in diamond. AVS Quantum Science **2**(2) (2020) https://doi.org/10.1116/5.0006785 https://pubs.aip.org/avs/aqs/article-pdf/doi/10.1116/5.0006785/13962349/024701_1_online.pdf. 024701

[9] Seif, A., Landsman, K.A., Linke, N.M., Figgatt, C., Monroe, C., Hafezi, M.: Machine learning assisted readout of trapped-ion qubits. Journal of Physics B: Atomic, Molecular and Optical Physics **51**(17), 174006 (2018) https://doi.org/10.1088/1361-6455/aad62b

[10] Luo, L., Xiong, Y., Liu, Y., Sun, X.: Adaptive Gradient Methods with Dynamic Bound of Learning Rate (2019)

[11] Davis, M.G., Smith, E., Tudor, A., Sen, K., Siddiqi, I., Iancu, C.: Towards optimal topology aware quantum circuit synthesis. In: 2020 IEEE International Conference on Quantum Computing and Engineering (QCE), pp. 223–234 (2020). https://doi.org/10.1109/QCE49297.2020.00036