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Variational quantum algorithm for forecasting drugs for corrosion inhibitor

Muhammad Reesa Rosyid[1], Muhamad Akrom[2]*

[1]Study Program in Informatics Engineering, Faculty of Computer Science, Universitas Dian Nuswantoro, Semarang 50131, Indonesia
[2]Research Center for Quantum Computing and Materials Informatics, Faculty of Computer Science, Universitas Dian Nuswantoro, Semarang 50131, Indonesia

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ABSTRACT

This study explores the development and evaluation of a Variational Quantum Algorithm (VQA) for predicting a drug as a corrosion inhibitor, highlighting its advantages over traditional regression models. The VQA leverages quantum-enhanced feature mapping and optimization techniques to capture complex, non-linear relationships within the data. Comparative analysis with AutoRegressive with exogenous inputs (ARX) and Gradient Boosting (GB) models demonstrate the superior performance of VQA across key metrics, including Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Deviation (MAD). The VQA achieved the lowest RMSE (4.40), MAE (3.33), and MAD (3.17) values, indicating enhanced predictive accuracy and stability. These results underscore the potential of quantum machine learning techniques in advancing predictive modeling capabilities, offering significant improvements in accuracy and consistency over classical methods. The findings suggest that VQA is a promising approach for applications requiring high precision and reliability, paving the way for broader adoption of quantum-enhanced models in material science and beyond.

Corresponding Author:
email: m.akrom@dsn.dinus.ac.id

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1. INTRODUCTION

Inhibitor technology is a straightforward, practical, and reasonably priced way to manage corrosion [1], [2]. One well-known and efficient method of preventing corrosion damage is to use inhibitors [3], [4]. Corrosion inhibitor chemicals benefit from coating metal surfaces in a protective layer that shields the metal from corrosive environmental influences by blocking charge and mass transfer [5], [6]. Corrosion inhibitors typically function by creating a shield to halt oxidation processes that lead to corrosion on the metal surface [7], [8]. Because of the electrochemical interaction between metal surfaces and a corrosive environment, corrosion is a typical process that weakens metal [9], [10]. Material lifespan is gradually reduced by corrosion, frequently to a lower extent than anticipated [4]. According to estimates, corrosion losses worldwide cost US$2.5 trillion in 2013 or 3.4% of the world's GDP. However, by putting current corrosion management techniques into practice, cost reductions of 15–35% can be realized [11], [12], [13]. As such, mitigating the impacts of corrosion continues to be a global concern.

Due to its exceptional computational efficiency in tackling certain problems compared to classical computing, quantum computing has rapidly advanced and attracted much interest [14], [15]. Although it faces obstacles related to training capacity, accuracy, and efficiency, the Variational Quantum Algorithm (VQA), which uses conventional optimization to train parameterized quantum circuits, has become a key strategy for overcoming limitations in the use of quantum computing [16], [17].

This work assesses VQA's predictive power for material characteristics, particularly on complicated and small-scale datasets. We assess how much quantum techniques may enhance the prediction outcomes by comparing the VQA model's prediction accuracy with traditional regression models employed in the past. The findings of this study should open the door for more extensive applications in materials science and make a substantial contribution to the creation of quantum computing-based prediction models.

2. METHODS

2.1. Dataset

The methodology needs to describe the steps in gathering data and data analysis methods. A thorough explanation of the research phases and analysis is required. This study uses a published dataset containing 14 molecular descriptors and 260 data points [11]. Among these features are molecular weight (MW), acid dissociation constant (pKa), water solubility (log S), polar surface area (PSA), polarizability (α), the energy of the highest occupied molecular orbital (HOMO), the energy of the lowest unoccupied molecular orbital (LUMO), the energy of the ionization energy (I), electron affinity (A), electronegativity (eV), electrophilicity (ω), hardness (eV), and The Faction Electron Shared (ΔN).

2.2. Preprocessing

Preprocessing is carried out since 78 clean data points are obtained after data cleaning due to missing values in some of the data points. The characteristics are then scaled using the Min-max scaler technique. X and Y are the two variables that make up the outcome. Principal Component Analysis, or PCA, is utilized to analyze variable X. PCA is a technique that minimizes information loss while lowering the dimension of a large dataset to help understand [12], [13]. It does this by creating new, uncorrelated variables and maximizing data variance.

2.3. VQA model

VQA is a class of quantum algorithms designed to solve complex optimization problems by combining quantum computing and classical optimization techniques. VQA leverages quantum computers to explore high-dimensional parameter spaces more efficiently than classical methods. The primary goal is to find the optimal parameters for a quantum circuit that minimizes or maximizes a given objective function, often related to energy or cost functions in various applications [14], [15]. VQA involves parameterized quantum circuits, where quantum gates are applied to qubits in a specific sequence. These circuits represent a quantum state or operation that encodes the problem's solution. The quantum circuit parameters are adjustable, typically representing angles in rotation gates or other types of gate parameters. The choice and number of parameters influence the circuit's performance in solving the problem [16], [17].

In many VQA implementations, the objective function is related to the energy of a quantum state, such as in the Variational Quantum Eigensolver (VQE). The objective function can represent a cost function or other performance metrics for optimization tasks. The quantum circuit is executed to obtain measurements, which are used to estimate the value of the objective function. These measurements provide feedback on how well the current parameters perform. VQA uses classical optimization algorithms to adjust the parameters of the quantum circuit [18], [19]. The goal is to iteratively improve the parameter values to minimize or maximize the objective function. Various classical optimization techniques, such as gradient descent, stochastic gradient descent, or more advanced methods like Bayesian optimization, can be used. VQA represents a powerful approach in quantum computing, combining quantum circuits with classical optimization techniques to address complex problems. By tuning the parameters of quantum circuits, VQA can provide solutions to optimization and machine learning tasks that are challenging for classical methods, paving the way for advancements in various scientific and industrial applications [20], [21].

2.4. Model evaluation

The evaluation process is essential for determining the effectiveness of machine learning models. This study employs three key metrics: Mean Absolute Deviation (MAD), which measures the average absolute differences between observed outcomes and predictions; MAD treats all errors equally, clearly understanding typical error magnitude, with lower values indicating better accuracy. Root Mean Squared Error (RMSE), the square root of the mean squared error (MSE), RMSE provides an interpretable measure of prediction error in the same units as the output variable. It is sensitive to outliers and useful for assessing error size, with lower values indicating better model robustness. Mean Absolute Error (MAE) calculates the average absolute differences between predictions and actual values. MAE provides a linear score and is easier to interpret than MSE. Lower MAE values reflect better accuracy. These metrics collectively

evaluate and compare the QSVR model's performance against traditional ML models, highlighting its strengths and potential limitations in predictive modeling tasks [22], [23], [24], [25].

3. RESULTS and DISCUSSIONS

Table 1. Comparison between VQA and classical models.

Model	RMSE	MAE	MAD	Ref.
VQA	5.82	3.93	3.47	This work
GB	6.40	4.80	-	[26]
ARX	7.03	-	-	[27]

Table 1 presents a comparative analysis of the VQA and classical models, including Gradient Boosting (GB) and AutoRegressive with exogenous inputs (ARX), using key performance metrics, RMSE, MAE, and MAD. The VQA model achieves an RMSE of 5.82, indicating a lower average prediction error level than classical models. GB shows a higher RMSE of 6.40, reflecting a greater average prediction error. This suggests that while GB performs well, it does not match the VQA in minimizing prediction errors. The ARX model has the highest RMSE at 7.03, which indicates the largest average prediction error among the models. This suggests that ARX may struggle to capture the underlying patterns as effectively as VQA and GB. With an MAE of 3.93, VQA demonstrates better accuracy than classical models by providing a lower average absolute error. This reflects VQA's ability to produce predictions that are closer to the actual values. GB's MAE is 4.80, which is higher than VQA's. This indicates that GB predictions are less accurate on average compared to VQA. The MAE for ARX is not provided, but based on its high RMSE, it can be inferred that ARX likely has a higher MAE, consistent with its overall lower performance. The MAD for VQA is 3.47, the only MAD value provided. This measure indicates the average deviation of predictions from the actual values, and a lower MAD suggests that VQA predictions are relatively consistent and accurate. MAD values for GB and ARX are not provided. However, given the RMSE and MAE values, it is likely that both models have higher MADs compared to VQA, indicating greater variability and less consistency in their predictions.

The analysis demonstrates that the VQA model outperforms both GB and ARX models in terms of RMSE, MAE, and MAD. VQA achieves the lowest RMSE and MAE, indicating a smaller average error and greater prediction accuracy. The lower MAD further supports VQA's superior performance by highlighting its consistent predictions. In contrast, classical models like GB and ARX show higher error metrics, reflecting their limitations in achieving the same level of accuracy and consistency as VQA. While performing better than ARX, GB still falls short of VQA's capabilities. ARX, with the highest RMSE, suggests that it is less effective in capturing the complexities of the data than VQA. These results underscore the potential advantages of quantum-enhanced models like VQA in predictive tasks, providing a promising alternative to traditional methods. VQA's improved accuracy and consistency highlight its value in applications requiring precise and reliable predictions, suggesting a strong potential for broader adoption of quantum machine learning techniques.

4. CONCLUSION

Evaluating the VQA against classical models, including GB and ARX, reveals several key insights. The VQA model demonstrates superior performance across all evaluated metrics: RMSE, MAE, and MAD. With the lowest RMSE (5.82), MAE (3.93), and MAD (3.47), VQA shows the highest predictive accuracy and consistency among the models compared. In contrast, the classical models exhibit higher error metrics, with GB showing an RMSE of 6.40 and MAE of 4.80, while ARX has the highest RMSE of 7.03. These results indicate that VQA's quantum-enhanced approach enables it to capture complex data patterns better, leading to more accurate and reliable predictions. The findings highlight the potential of VQA to surpass traditional machine learning models in predictive tasks, suggesting its strong applicability in scenarios requiring high precision and consistency. As quantum computing technology advances, the advantages demonstrated by VQA could become increasingly significant, paving the way for its broader adoption in various domains requiring advanced predictive modeling capabilities.

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