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Harnessing Quantum SVR on Quantum Turing Machine for Drug Compounds Corrosion Inhibitors Analysis

Akbar Priyo Santosa[1], Muhammad Reesa[1], Lubna Mawaddah[1], Muhamad Akrom[2*]

[1]Study Program in Informatics Engineering, Faculty of Computer Science, Universitas Dian Nuswantoro, Jl. Imam Bonjol No.207 Semarang, Central Java 50131, Indonesia

[2]Research Center for Quantum Computing and Materials Informatics, Faculty of Computer Science, Universitas Dian Nuswantoro, Jl. Imam Bonjol No.207 Semarang, Central Java 50131, Indonesia

*m.akrom@dsn.dinus.ac.id

Abstract. Corrosion is an issue that has a significant impact on the oil and gas industry, resulting in significant losses. This is worth investigating because corrosion contributes to a large part of the total annual costs of oil and gas production companies worldwide, and can cause serious problems for the environment that will impact society. The use of inhibitors is one way to prevent corrosion that is quite effective. This study is an experimental study that aims to implement machine learning (ML) on the efficiency of corrosion inhibitors. In this study, the use of the *Quantum Support Vector Regression* (QSVR) algorithm in the ML approach is used considering the increasingly developing quantum computing technology with the aim of producing better evaluation matrix values than the classical ML algorithm. From the experiments carried out, it was found that the QSVR algorithm with a combination of (TrainableFidelityQuantumKernel, ZZFeatureMap/ PauliFeatureMap, and linear entanglement) obtained better Root Mean Square Error (RMSE) and model training time with a value of 6,19 and 92 compared to other models in this experiment which can be considered in predicting the efficiency of corrosion inhibitors. The success of the research model can provide a new insights of the ability of quantum computer algorithms to increase the evaluation value of the matrix and the ability of ML to predict the efficiency of corrosion inhibitors, especially on a large industrial scale.

Keywords: Corrosion, machine learning, *quantum computing*, *quantum support vector regression*, predictive analysis, machine learning efficiency

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1. Introduction

Corrosion is an electrochemical process between metal surfaces and corrosive environments, which can cause significant losses in various industries, especially in the oil and gas industry [1-3]. Corrosion is worth investigating, especially in oil field applications, as corrosion issues contribute to a significant portion of the annual costs of oil and gas production companies worldwide.

Additionally, proper corrosion protection can help avoid various potential disasters that could lead to serious issues such as loss of life, negative impacts on society, and pollution of water resources and the environment [4-6].

Among many corrosion control and prevention methods, the use of corrosion inhibitors is very common. Corrosion inhibitors are substances that reduce or prevent metal reactions with the corrosive environment when added in small concentrations [7-10]. Corrosion inhibitors generally consist of organic compounds whose molecules contain heteroatoms such as phosphorus (P), nitrogen (N), oxygen (O), sulfur (S), and arsenic (As), which can enable strong interactions between organic molecules and metal atoms in forming a protective layer on the metal surface absorbed at the corrosive metal solution interface due to the presence of free electrons in double bonds [11-14].

In its application, prevention is better than cure. Machine Learning (ML) can assist in this regard, but classical ML would take a long time to predict if the processed data is very large. In technological developments, Quantum Computing (QC) has attracted wide attention due to its unprecedented computational efficiency in solving specific problems compared to classical computation. As in recent research, it has been revealed that quantum computing can provide better evaluation results than classical computing within the limits of the same or similar problem topics and datasets [15-19].

In 1982, after Richard Feynman proposed his QC theory, Feynman argued that quantum problems could only be solved using QC [20]. In 1985, David Deutsch provided a new perspective on computation by developing the Quantum Turing Machine (QTM) [21]. Unlike ordinary classical Turing machines, QTM employs quantum mechanics principles, opening up new phenomena such as superposition. For example, if a classical Turing machine processes a step-by-step algorithm model, then QTM will execute the algorithm model as a whole where many calculations can be done simultaneously. We can still study this phenomenon with ordinary classical Turing machines and QTM which are still being developed [22].

In this study, an investigation is conducted by applying the Quantum Support Vector Regression (QSVR) algorithm on the Quantum Turing Machine (QTM) to study the regression of pharmaceutical compounds as corrosion inhibitors. This approach evaluates several aspects, including model training ability, accuracy measured using the R2 matrix, Mean Absolute Error (MAE), Mean Square Error (MSE), Root Mean Square Error (RMSE), and computational efficiency by measuring execution time. Those evaluations are to measure the results of how the ML works.

2. Methods

2.1. Dataset

This study uses a published dataset containing 260 data points with 14 molecular descriptors [22]. These features include molecular weight (MW), acid dissociation constant (pKa), octanol-water partition coefficient (log P), water solubility (log S), polar surface area (PSA), polarizability (α), energy of highest occupied molecular orbital (E-HOMO), energy of lowest unoccupied molecular orbital (E-LUMO), Ionization Energy (I), Electron Affinity (A), Electronegativity (eV), Electrophilicity (ω), Hardness (eV), and The Faction Electron Shared (ΔN). All those features to calculate the overall inhibitor efficiency in general.

2.2. Preprocessing

The preprocessing stage is performed because some data points have missing values, resulting in data cleaning with 78 clean data points. Then, feature scaling is performed using the Min-max scaler method, which will then be divided into variables X and y. In variable X, Principal Component Analysis (PCA) is performed. PCA is a technique that reduces the dimension of a large dataset to facilitate interpretation while minimizing information loss by creating new variables that are uncorrelated and maximizing data variance [23]. Thus, it simplifies data complexity without reducing important information in the dataset. With PCA, features are reduced to the 5 most

significant features while retaining 95% of the data information. PCA was chosen to make model execution more time efficient because some features were pruned. Next, the data is divided into training and testing data sets to validate the model's performance on data not involved in the training process, thus reducing overfitting, and divided into 80% training data and 20% testing data.

2.3. ML Model

In this case study, the ML model uses the *Quantum Support Vector Regression* (QSVR) algorithm, where QSVR itself is a development of the classical Support Vector Regression (SVR) algorithm. In this implementation, some aspects are combined in ML to obtain the best results, including Quantum Kernel, Feature map, and entanglement influence, as shown in Figure 1. In the initial experiment, the clean data input is transformed from classical to quantum input with a quantum map. Then it will be processed by calling functions from the quantum kernel, which will then be trained and evaluated following the steps as shown in Figure 2.

A quantum kernel is a kernel that has a positive definite symmetric conjugate function κ that maps two variables $x, y \in X$ to a complex space, $\kappa: X \times X \rightarrow C$. The function of the quantum kernel must meet the kernel function requirements and can be evaluated by a quantum computer. The important result of the kernel function is known as the kernel trick, which depends on the fact that any kernel function can be written as a product in the potentially high-dimensional feature space, $\kappa(x, y) = \varphi\dagger(x)\varphi(y)$ [24].

The feature map used is a quantum map that takes a Hilbert space representation that states that the quantum state of n qubits will result in a 2n-dimensional space, where the quantum state can encompass superposition and entanglement [25]. This experiment uses several feature maps such as ZZFeatureMap, Pauli Feature Map, and ZfeatureMap as shown in Figures 3 and 4. Those feature maps are some features of the Qiskit library to change data from classical numeric to quantum data that is by the QSVR algorithm.

Entanglement is a state where the quantum system and particles at each point are interconnected and inseparable. If the quantum state of a composite system cannot be directly expressed as a direct product of the quantum state of two combined subsystems, then the pure state of the system can be either a pure quantum state or an entangled state [26]. This study uses "linear" entanglement because this feature is most suitable for the combination of QSVR algorithms, to find out whether the entanglement feature can produce a better evaluation matrix.

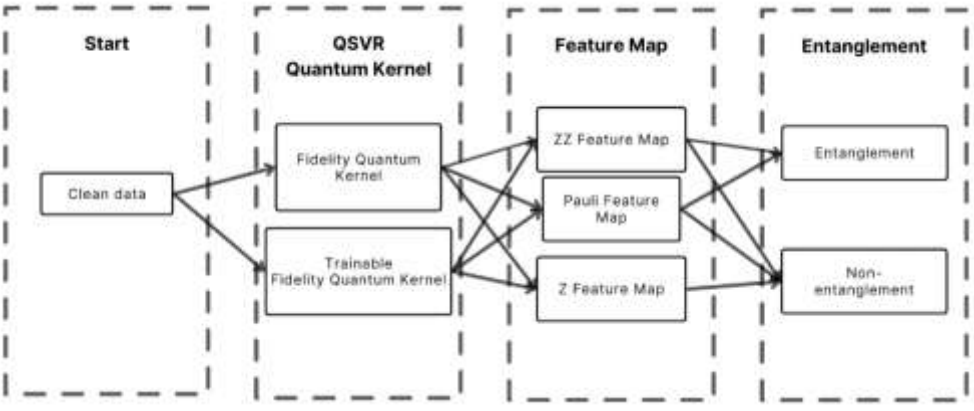

Figure 1. ML model combination

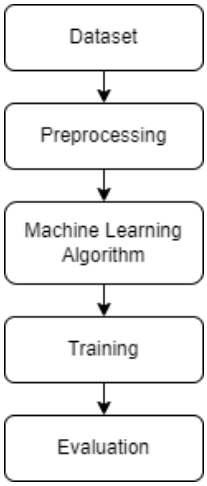

Figure 2. Work steps

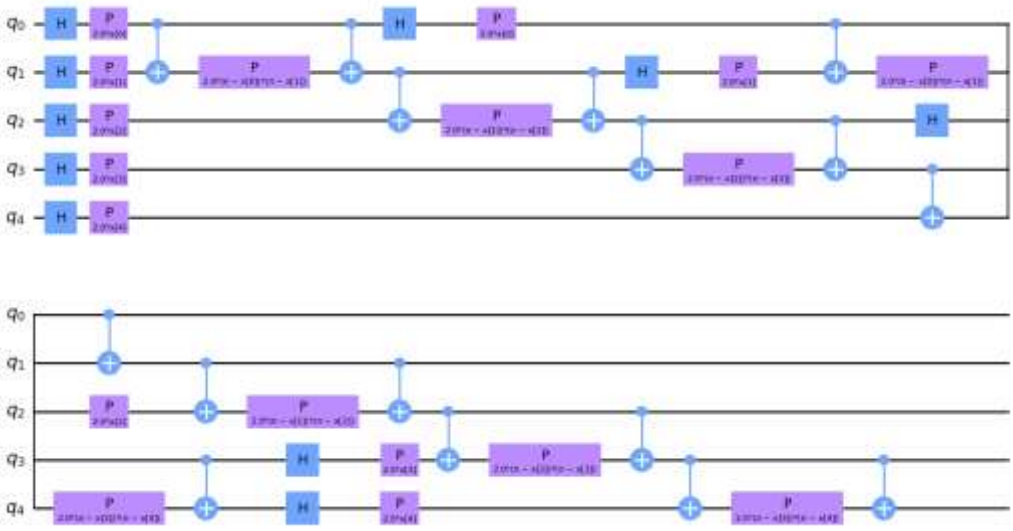

Figure 3. ZZFeatureMap dan PauliFeatureMap

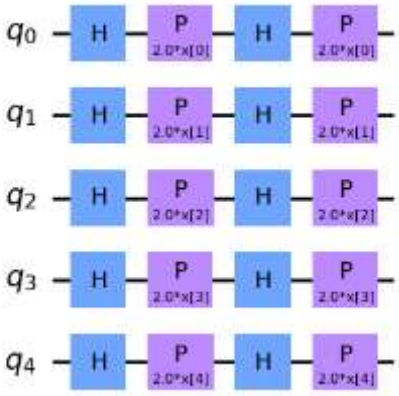

Figure 4. ZFeatureMap

Table 1. Model parameter

Model	Kernel	Feature Map	Entanglement
Model01	FidelityQuantumKernel	ZZFeatureMap	Linear
Model02			Non-entanglement
Model03		PauliFeatureMap	Linear
Model04			Non-entanglement
Model05		ZFeature Map	Non-entanglement
Model06	TrainableFidelityQuantumKernel	ZZFeatureMap	Linear
Model07			Non-entanglement
Model08		PauliFeatureMap	Linear
Model09			Non-entanglement
Model10		ZFeature Map	Non-entanglement

2.4 Evaluation

Evaluation is carried out to determine a good ML model through a comparison of the experiment results conducted in Table 1. Evaluation in this case study uses several matrices such as R2, MSE, RMSE, MAE, and model training time [27]. This evaluation matrix is used because it is often and commonly used in the evaluation of ML models in regression cases to determine the performance of the ML model.

3. Results and Discussion

Table 2. Experiment Results

Model	R^2	MAE	MSE	RMSE	Training time
Model01	-0,16	4,93	38,32	6,19	102
Model02	-0,18	4,88	38,92	6,24	100
Model03	-0,16	4,93	38,32	6,19	100
Model04	-0,18	4,88	38,92	6,24	92
Model05	-0,25	5,07	41,13	6,41	227
Model06	-0,16	4,93	38,32	6,19	92
Model07	-0,18	4,88	38,92	6,24	93
Model08	-0,16	4,93	38,32	6,19	92
Model09	-0,18	4,88	38,92	6,24	94
Model10	-0,25	5,07	41,13	6,41	92

The results of experiments with various combinations of ML models from Table 1 are then presented in the evaluation matrix shown in Table 2. The presented experiment results showcase the performance of ten distinct machine learning (ML) models, denoted as Model01 to Model10, in a regression task. Various evaluation metrics such as R2 (coefficient of determination), MAE (mean absolute error), MSE (mean squared error), and RMSE (root mean squared error) are utilized to assess the efficacy of these models. Additionally, the training time for each model is recorded.

The MAE and RMSE values across all models range from 4.88 to 5.07 and from 6.19 to 6.41, respectively. Despite the negative R2 values observed in all models, indicating poor fit to the data and was obtained due to the combination of ML models that were not yet suitable and needed further development, other evaluation metrics yield noteworthy results. These findings suggest that while

the models may not explain the variance in the data adequately, they still provide relatively accurate predictions, as indicated by the low MAE and RMSE values.

Moreover, an intriguing observation arises from Models 01, 03, 06, and 08, which exhibit entanglement during the training process. Entanglement, a phenomenon rooted in quantum mechanics, has been proposed as a mechanism to enhance ML model performance. The presence of entanglement in these models suggests a potential avenue for improving predictive accuracy, albeit further investigation is warranted.

Furthermore, the considerable disparity in model training times underscores the ongoing development of quantum computation. Despite advancements in quantum computing technologies, the training times remain inefficient for practical applications. This highlights the current limitations in harnessing quantum computing power for complex ML tasks.

In conclusion, the experiment results highlight the performance and potential of ML models in regression tasks, emphasizing the significance of alternative methodologies such as quantum entanglement. These findings suggest that refining quantum computing techniques could unlock its full potential in enhancing ML model performance. Future research should focus on advancing these quantum methods to further improve ML outcomes.

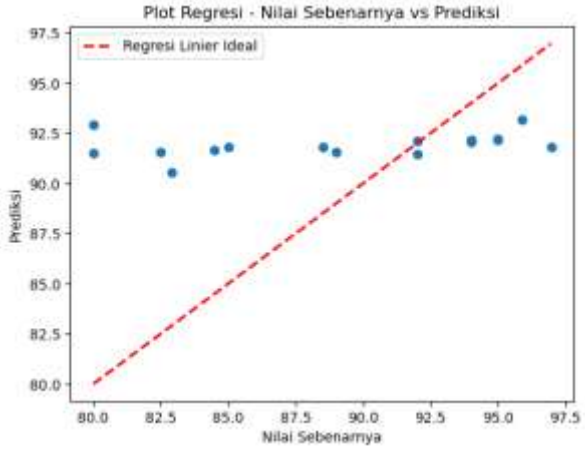

Figure 5. Graph of the prediction results of Model06 and Model08

4. Conclusion

For the regression study of drug compounds as corrosion inhibitors, considering the RMSE value and model training time, Model06 and Model08 can be proposed as superior ML models. In the combination of these models, the selection of quantum kernel and entanglement usage can enhance the evaluation results. The results of this experiment can be used as a learning experience and additional reference on how to solve regression cases with the QSVR algorithm, which is relatively new and can be an option in solving regression cases, especially on a large scale. However, this study needs to be improved. Optimization in the selection of ML combinations such as quantum kernels can be one way to achieve better results, especially in terms of efficiency, particularly model training time. Therefore, further research is needed so that the overall evaluation matrix results of the models can yield better values.

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