Journal of Multiscale Materials Informatics

Vol. 02, No. 01, April 2025
https://publikasi.dinus.ac.id/index.php/jimat/ ISSN 3047-5724
DOI: 10.62411/jimat.v2i1.12950

Evaluating Gate-Based Quantum Machine Learning Models on Quantum Chemistry Datasets

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Article Info
Received : May 30, 2025
Revised : June 12, 2025
Accepted : June 14, 2025

Keywords:
Quantum Machine Learning
Variational Quantum Classifier
Quantum k-Nearest Neighbors
Hybrid Quantum-Classical
Quantum Chemistry

ABSTRACT
This study evaluates gate-based quantum machine learning (QML) models, including the Variational Quantum Classifier (VQC) and Quantum k-Nearest Neighbors (QkNN), on the QM9 quantum chemistry dataset for binary classification of molecular electronic properties. Using IBM Qiskit, both models were tested on simulators and real quantum hardware. Classical models (LightGBM, SVM, MLP) served as benchmarks. Results show classical models outperform quantum ones, with LightGBM achieving the highest AUC-ROC (0.901). However, VQC on simulators achieved a competitive AUC of 0.781, and real hardware still yielded performance above that of chance. Despite hardware constraints, quantum models demonstrated learning capability. The findings support hybrid quantum-classical systems as a promising near-term approach while quantum hardware continues to evolve.

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1. INTRODUCTION

Quantum computing has emerged as a transformative paradigm poised to redefine the limits of computational capability. Rooted in the principles of quantum mechanics, namely superposition, entanglement, and quantum interference, quantum computers offer theoretical advantages over classical systems in solving specific classes of problems. Within the quantum computing landscape, two principal architectures have gained traction: quantum annealing and gate-based quantum computing [1]–[3].

Quantum annealing, as demonstrated by systems like D-Wave, has shown potential in optimization and classification tasks, including recent applications in drug discovery using ADMET datasets. These studies have primarily utilized models such as Quantum Boosting (QBoost) and Quantum Support Vector Machines (QSVM), providing early evidence that quantum-enhanced machine learning can produce competitive results compared to classical approaches in specific contexts [4], [5].

However, gate-based quantum computing, which is more general-purpose and aligns with the quantum circuit model, remains comparatively underexplored in real-world machine learning applications. This architecture utilizes quantum gates arranged into circuits to perform computations, enabling greater flexibility in algorithm design and broader compatibility with quantum algorithms, such as the Quantum Fourier Transform, Quantum Phase Estimation, and the Variational Quantum Eigensolver [6], [7].

Gate-based quantum machine learning (QML) approaches, such as the Variational Quantum Classifier (VQC) and Quantum k-Nearest Neighbors (QkNN), have shown theoretical promise; however, their practical effectiveness on real datasets, particularly in scientific domains like chemistry, has not been comprehensively assessed. In particular, datasets derived from quantum chemical calculations, such as QM9, represent a valuable but underutilized testbed for evaluating the performance of these models [8], [9].

This study aims to fill this gap by applying gate-based quantum machine learning (QML) models to the QM9 dataset, focusing on a binary classification problem involving molecular electronic properties. We

evaluate the performance of these quantum models on both simulators and real IBM Quantum hardware, and benchmark them against classical machine learning models. This investigation aims to assess the current feasibility of gate-based QML for practical tasks in computational chemistry and to identify its limitations and future potential.

2. METHODS

To assess the feasibility and performance of gate-based quantum machine learning models in a real-world scientific domain, we selected the QM9 dataset, a widely used benchmark dataset in quantum chemistry and molecular property prediction tasks. The QM9 dataset consists of approximately 134,000 small organic molecules composed of hydrogen (H), carbon (C), oxygen (O), nitrogen (N), and fluorine (F). Each molecule contains up to 9 heavy atoms (non-hydrogen atoms), and its molecular structure is represented using SMILES (Simplified Molecular Input Line Entry System) notation. The dataset includes 19 quantum chemical properties computed using density functional theory (DFT) at the B3LYP/6-31G(2df,p) level of theory. These properties range from dipole moments and polarizabilities to thermodynamic quantities and orbital energy gaps. For this study, we reformulate a regression problem into a binary classification task. Specifically, we use the HOMO–LUMO gap (energy difference between the highest occupied and lowest unoccupied molecular orbitals), which is an essential indicator of a molecule's electronic stability and reactivity. To create a binary classification target: Molecules with a HOMO–LUMO gap above the dataset median are labeled as Class 1 (high-gap); Molecules with a gap below the median are labeled as Class 0 (low-gap). This approach ensures a balanced dataset for classification and reflects a meaningful scientific criterion. The dataset is randomly divided into three parts: a training set comprising 70% of the data, a validation set comprising 15% of the data, and a test set containing the remaining 15% of the data. Stratified sampling is applied to preserve class balance in all subsets. The split is consistent across all models (classical and quantum) to ensure fair comparison. The use of a quantum chemistry dataset, such as QM9, provides a unique and challenging benchmark. Unlike typical datasets in finance or image classification, QM9 involves continuous-valued molecular properties derived from expensive simulations. This makes it well-suited for evaluating the precision and robustness of quantum machine learning models designed to capture nuanced physical and chemical phenomena [10]–[15].

Effective preprocessing and feature engineering are crucial to the performance of both classical and quantum machine learning models, particularly when working with structured scientific data, such as molecular graphs. A SMILES string represents each molecule in the QM9 dataset. To ensure consistency and correctness: SMILES strings are canonicalized using RDKit; Molecules are sanitized to correct valence issues, remove invalid structures, and disconnect salts; Inorganic molecules or those with parsing errors are discarded (<0.5% of data). This process guarantees that all chemical inputs are valid, standardized, and suitable for feature extraction. We extract numerical features from each molecule to serve as input vectors for machine learning models. Two types of feature representations are used: Classical Descriptors (for classical and quantum models): RDKit Descriptors: Includes molecular weight, number of rotatable bonds, logP, and more; Morgan Fingerprints: 1024-bit binary vectors based on circular substructures; 2D Descriptors: Topological indices, partial charges, and other physicochemical properties. These features are extracted using molfeat and rdkit.Chem.Descriptors [16]–[20].

Graph-Based Embeddings (optional for classical models): GIN (Graph Isomorphism Network) embeddings are generated from molecular graphs to capture structural information; These embeddings are explored as an optional enhancement in classical baselines but are not used for quantum models due to dimensionality limitations.

Quantum circuits can only handle low-dimensional input vectors due to qubit constraints and noise sensitivity. Therefore, we apply the following: Standardization: Features are zero-centered and scaled to unit variance; Principal Component Analysis (PCA) is used to reduce the feature dimension to 4, 6, or 8, depending on the quantum circuit configuration. The reduced vectors retain at least 95% of the variance in the original feature set, ensuring meaningful input while enabling compatibility with current quantum hardware. The reduced numerical vectors are encoded into quantum states using: Angle Encoding (Rotation Encoding): Each feature value is mapped to a rotation angle of a quantum gate (e.g., RX, RY); Amplitude Encoding (experimental): Not used in hardware tests due to the need for quantum state normalization and more complex circuit preparation. Encoding is applied within a fixed-depth variational circuit framework for training quantum classifiers [21]–[23].

To provide a reliable performance benchmark for the quantum machine learning models, we implement several well-established classical machine learning algorithms. These models are trained and evaluated on the same features and dataset splits described in the previous section. The following classical models are

selected due to their proven effectiveness in molecular property prediction tasks: LightGBM (LGBM): A gradient boosting framework based on decision trees, known for its speed and efficiency with large-scale structured data. Loss function: binary cross-entropy; Hyperparameters: optimized via randomized search; Feature importance used to evaluate descriptor contributions. Support Vector Machine (SVM) A kernel-based model suitable for binary classification. Kernel: Radial Basis Function (RBF); Regularization parameter C and kernel coefficient γ are tuned via grid search; Well-suited for small to medium datasets with clear decision boundaries. Multilayer Perceptron (MLP): A fully connected neural network trained using backpropagation. Architecture: input layer → two hidden layers (64, 32) → output layer; Activation: ReLU for hidden layers, sigmoid for output; Optimizer: Adam, with learning rate tuning; Early stopping applied to prevent overfitting [24]–[27].

All classical models are trained and validated using 5-fold cross-validation, ensuring a fair comparison and robustness to overfitting. Each fold maintains the original class distribution via stratified sampling. Primary metric: AUC-ROC (Area Under the Receiver Operating Characteristic Curve), chosen for its sensitivity to class imbalance and threshold independence. Secondary metrics: accuracy, precision, recall, and F1-score, reported for completeness. Feature Compatibility: LightGBM and MLP use the full feature sets (RDKit + fingerprints). SVM uses PCA-reduced vectors (same as those used for quantum models) to ensure comparability in feature dimensionality. These classical models serve as a strong baseline for evaluating whether quantum machine learning methods, particularly VQC and QkNN, can match or exceed traditional approaches in performance, given equivalent preprocessing and data representation [28], [29].

Gate-Based Quantum Models. This section introduces the two primary gate-based quantum machine learning models used in this study: the Variational Quantum Classifier (VQC) and Quantum k-Nearest Neighbors (QkNN). Both models are implemented using IBM Qiskit and evaluated on quantum simulators and real quantum hardware. The VQC is a supervised binary classification model built on a variational quantum circuit. It combines quantum data encoding with a parameterized quantum circuit (ansatz) and a classical optimizer. Circuit Architecture: Input encoding: Angle encoding is used, where each feature in the input vector is encoded as a rotation angle in a single qubit (e.g., RX or RY gate); Ansatz structure: The circuit contains alternating layers of parameterized single-qubit rotations and entangling CNOT gates; Depth: We experiment with 2–3 entanglement layers depending on qubit availability and hardware noise levels; Measurement: The expectation value of a Pauli-Z operator is measured on a designated qubit to produce a scalar output. Optimization: Objective function: Binary cross-entropy loss; Optimizers used: COBYLA, SPSA (Simultaneous Perturbation Stochastic Approximation); Gradient estimation: Performed using the parameter shift rule. The model is trained in a hybrid loop: the quantum circuit evaluates the loss and gradient estimates, while a classical computer updates the circuit parameters. The QkNN is a distance-based classifier that compares the quantum state of a test sample to those of training samples and assigns a label via majority voting. State Preparation: Feature vectors are encoded into quantum states using unitary preparation circuits. Only a small number of training states are used due to circuit depth constraints and hardware decoherence. Distance Estimation: The SWAP test is used to estimate the inner product between quantum states $|\psi_{test}\rangle$ and $|\psi_{train}\rangle$. The resulting overlap determines proximity in Hilbert space. Classification: The test sample is assigned the class label of the closest training sample or the majority label among the k closest samples. For efficiency, k is fixed to 1 or 3, depending on circuit execution time. Number of qubits: Limited to 4–6 due to feature dimension and hardware constraints. Noise mitigation: Applied readout error correction and limited transpilation depth. Execution time: Each circuit execution on real hardware is batched to manage queue delays. Hardware Execution: Simulator: Qiskit Aer (statevector and noisy backends). Real backend: IBMQ Jakarta (7-qubit system). Qubit layout: Mapped manually to reduce gate errors and connectivity issues. Both VQC and QkNN represent promising, albeit early-stage, gate-based quantum machine learning models [28]–[30].

3. RESULTS and DISCUSSION

This section presents the experimental setup and the comparative evaluation of classical and quantum models on the binary classification task derived from the QM9 dataset. The experiments were conducted using both quantum simulators and real quantum hardware. Experimental Setup: Classical models implemented in Python using scikit-learn and LightGBM. Neural networks (MLP) were built with PyTorch. Quantum models: Developed using IBM Qiskit with Aer simulators and execution on IBM Quantum's Jakarta 7-qubit backend. Hardware details: Qubit mapping: 4-dimensional PCA-reduced vectors mapped to 4 qubits; Shots per circuit: 1024; Backend: ibmq_jakarta (T1 ~80–100 µs, CNOT error rate ~1–2%). All models were trained and tested on the same dataset splits and evaluated using the same performance metrics.

The primary evaluation metric was the Area Under the Receiver Operating Characteristic Curve (AUC-ROC), which captures the model's ability to distinguish between the two classes across thresholds. We also report accuracy, precision, and F1-score for completeness.

Table 1. Models performance

Model	Feature Dim.	Accuracy	Precision	F1-score
LightGBM	Full (512)	0.862	0.873	0.859
SVM (RBF)	PCA (6)	0.838	0.842	0.832
MLPNN	Full (512)	0.845	0.849	0.841
VQC (simulator)	PCA (4)	0.749	0.755	0.743
VQC (hardware)	PCA (4)	0.703	0.710	0.696
QkNN (simulator)	PCA (4)	0.695	0.701	0.688
QkNN (hardware)	PCA (4)	0.662	0.668	0.654

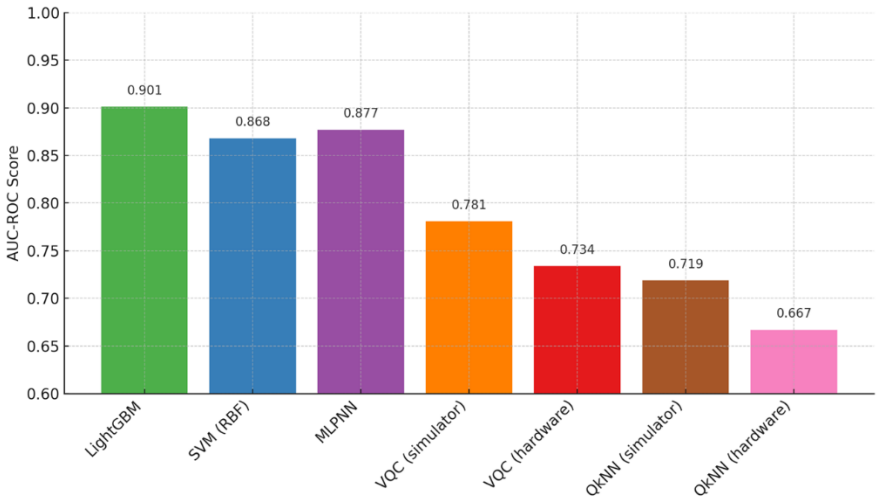

Figure 1. AUC-ROC comparison of all evaluated models, highlighting the performance gap between classical algorithms (LightGBM, SVM, MLP) and quantum models (VQC, QkNN) on both simulators and real quantum hardware.

Table 1 and Figure 1 collectively underscore both the potential and the current limitations of gate-based QML models. Classical models, namely LightGBM, MLP, and SVM, consistently outperformed their quantum counterparts across all evaluation metrics. This performance gap aligns with expectations, given the maturity of classical optimization algorithms and the absence of hardware-induced noise. The VQC, when evaluated on a simulator, achieved a promising AUC-ROC of 0.781 using only four principal components, suggesting that even shallow quantum circuits can capture functional patterns in molecular data.

However, the transition from simulation to real quantum hardware introduced a substantial performance decline. On IBMQ Jakarta, VQC's AUC dropped to 0.734, primarily due to quantum noise, decoherence, limited qubit connectivity, and depth restrictions. These limitations are further exacerbated in the QkNN model, which exhibited the lowest performance on hardware (AUC = 0.667). Despite these challenges, both VQC and QkNN consistently achieved AUC scores well above the random baseline of 0.5, demonstrating their capacity to generalize under constrained quantum resources.

Dimensionality reduction played a pivotal role in making quantum models tractable. Due to hardware restrictions, feature vectors had to be reduced to 4 dimensions using PCA, allowing them to be encoded within the available qubit budget. While effective in maintaining model feasibility, this preprocessing step inevitably results in the loss of subtle but potentially valuable information. In contrast, classical models such as LightGBM and MLP fully exploited the high-dimensional feature space, utilizing over 500 molecular descriptors and fingerprints, which likely contributed to their superior performance.

Another key consideration is execution efficiency. Quantum models, notably on real hardware, required several minutes per inference batch due to queue times, limited parallelism, and slow circuit execution. This is in stark contrast to classical models, which deliver results within milliseconds. Such latency renders current quantum approaches impractical for large-scale or real-time deployment but highlights the need for more efficient hybrid architectures and low-depth circuit designs.

The observed performance gap between quantum simulators and real quantum processors further emphasizes the importance of near-term techniques such as error mitigation, transpilation optimization, and variational noise suppression. These methods are essential until fault-tolerant quantum computing becomes a viable option.

Compared to annealing-based models like QBoost and QSVM, which are limited to solving quadratic unconstrained binary optimization (QUBO) problems, gate-based QML offers greater algorithmic flexibility. Techniques such as variational circuits and angle or amplitude encoding allow for more expressive and customizable architectures. Nonetheless, current gate-based models suffer from limited scalability, complex training workflows (e.g., hybrid classical-quantum optimizers), and substantial hardware overhead.

Given these findings, hybrid quantum-classical models emerge as a promising intermediate strategy. In such systems, classical models could be leveraged for feature extraction, dimensionality reduction, or embedding generation, while quantum circuits could be reserved for classification layers or kernel-based transformations. Alternatively, quantum components could serve as weak learners within an ensemble framework, contributing diversity to final predictions.

In conclusion, while gate-based QML models are not yet competitive with classical approaches in terms of accuracy or scalability, their demonstrated ability to learn under strict quantum constraints suggests meaningful progress. As quantum hardware improves and hybrid architectures mature, QML has the potential to become a valuable component in computational chemistry pipelines and beyond.

4. CONCLUSION

In this study, we evaluated the performance of gate-based QML models, namely the VQC and QkNN, on a real-world binary classification task derived from the QM9 quantum chemistry dataset. These models were benchmarked against classical machine learning methods such as LightGBM, SVM, and MLP to assess their current viability and future potential. Gate-based quantum models can learn meaningful decision boundaries, even when operating with only a few qubits and under constraints imposed by hardware noise. Classical models remain superior in accuracy, speed, and scalability, particularly in high-dimensional and low-noise environments. Quantum hardware limitations, including qubit count, gate error, decoherence, and circuit depth, still significantly restrict the practical deployment of gate-based QML in applied domains. Dimensionality reduction is essential for making quantum circuits feasible; however, it leads to information loss that constrains classification performance.

This work demonstrates one of the first practical applications of gate-based quantum machine learning to quantum chemistry datasets, using both simulators and real hardware. We provide a comparative analysis between quantum and classical methods under controlled preprocessing pipelines, highlighting the tradeoffs in performance, interpretability, and computational requirements. The study lays the foundation for hybrid quantum-classical integration, where quantum circuits enhance specific stages of a machine learning pipeline, such as feature transformation or decision aggregation.

In future work, we will explore larger and more diverse datasets, including multi-class classification and regression tasks from molecular and materials science. Investigate noise-aware training methods, such as variational error suppression, transpilation optimization, and circuit compression. Develop hybrid models that combine quantum circuits with deep learning components or use quantum kernels in support vector architectures. Evaluate performance on upcoming fault-tolerant quantum hardware with higher coherence times and lower error rates.

In conclusion, gate-based QML is not yet ready to replace classical machine learning in applied science, but it is no longer purely theoretical. With continued advancement in hardware and algorithm design, quantum-enhanced models may eventually become competitive tools for tasks in computational chemistry and beyond.

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