



## Hybrid Quantum–Classical ML Systems for Complex Problem Solving

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### **Abstract:-**

Hybrid quantum–classical machine learning (HQC-ML) systems combine quantum computing primitives with classical machine-learning pipelines to address computationally hard problems. This paper reviews the current landscape of HQC-ML, surveys relevant literature, analyzes existing systems, and proposes a concrete hybrid architecture optimized for combinatorial optimization and high-dimensional data modeling. We present an experimental design and expected results comparing purely classical baselines against the proposed hybrid approach on representative problem classes (vehicle routing and molecular property prediction). The paper concludes with a discussion of limitations, implementation considerations, and future research directions.

**Keywords:** hybrid quantum–classical, variational quantum algorithms, quantum machine learning, combinatorial optimization, quantum feature maps

### **1. Introduction**

Quantum computing promises new ways to process information that can, for certain problem classes, offer computational advantages over classical approaches. However, current quantum hardware is noisy and limited in scale (NISQ era). Hybrid quantum–classical machine learning systems seek to leverage the strengths of both paradigms: quantum circuits for compact representation and exploration of complex solution spaces, and classical algorithms for data preprocessing, optimization orchestration, and robust inference. This hybridization allows near-term utility while sidestepping the need for fault-tolerant quantum processors [1,2].

This paper focuses on HQC-ML design principles, surveys empirical and theoretical developments, and describes a proposed system tailored to complex practical problems: combinatorial optimization (e.g., routing, scheduling) and high-dimensional scientific prediction (e.g., molecular



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property prediction). We aim to provide a reproducible experimental plan and clear performance targets to evaluate hybrid benefits.

## 2. Literature Survey

### 2.1 Quantum computing primitives relevant to ML

- **Variational Quantum Algorithms (VQAs):** Parameterized quantum circuits trained via classical optimizers. Examples include the Variational Quantum Eigensolver (VQE) and the Quantum Approximate Optimization Algorithm (QAOA). VQAs are the backbone of many HQC-ML approaches because they fit the NISQ setting [3].
- **Quantum Feature Maps and Kernel Methods:** Quantum circuits used to map classical data into high-dimensional Hilbert spaces to improve class separability. Quantum kernels can be evaluated on hardware and used within classical kernel methods (e.g., SVM).
- **Quantum Data Loading and Encodings:** Strategies to encode classical data into quantum states—amplitude encoding, basis encoding, angle encoding—each offering trade-offs between circuit depth and qubit count [4].

### 2.2 Hybrid quantum–classical training loops

Hybrid models typically alternate between quantum circuit evaluation and classical parameter updates. Classical optimizers (e.g., gradient-based, evolutionary strategies) interact with quantum subroutines to minimize loss functions. Techniques to mitigate barren plateaus and noise-aware training are active research areas.

### 2.3 Applications of HQC-ML

- **Combinatorial optimization:** QAOA and related variational approaches have been applied to MaxCut, traveling salesman variants, and vehicle routing problems. Evidence suggests promise for structured problems but scalability and noise sensitivity remain challenges.
- **Chemistry and material science:** VQE and hybrid workflows are used to approximate molecular ground states and energy surfaces; hybrid ML aids in feature extraction and surrogate modeling for quantum calculations.
- **Classification and regression:** Quantum kernels and variational classifiers have been benchmarked on standard datasets; results show mixed performance—advantages may appear for specific feature-structured datasets [5].

### 2.4 Open challenges

- **Noise and decoherence:** NISQ devices have limited circuit depth and high error rates.



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- **Scalability:** Encoding large classical datasets is expensive in qubit resources or circuit depth.
- **Optimization difficulties:** Barren plateaus, local minima, and optimizer mismatches hinder training.
- **Benchmarking and reproducibility:** Lack of standardized benchmarks and reliable baselines complicate assessment.

### 3. Existing Systems

We analyze representative HQC systems and frameworks along two dimensions: software stacks and end-to-end application deployments.

#### 3.1 Software frameworks

- **Qiskit (IBM):** Provides noise modeling, transpilation, and VQA/QAOA primitives. Strong hardware integration for IBM devices.
- **PennyLane (Xanadu):** Focused on differentiable quantum computing with tight integration to classical ML libraries (PyTorch, TensorFlow). Excellent for variational hybrid models.
- **Cirq (Google) and TensorFlow Quantum:** Emphasize low-level circuit control and quantum-classical integration for research-grade experimentation [6].

These frameworks enable prototyping but differ in abstraction level, device support, and ease of integrating classical ML components.

#### 3.2 Deployed hybrid applications

- **Quantum-assisted optimization pipelines:** Companies and research groups have implemented hybrid solvers where QAOA provides candidate moves inside classical metaheuristics (e.g., tabu search, simulated annealing). The quantum component is typically used to explore hard-to-reach regions of solution space.
- **Chemical property prediction workflows:** Hybrid systems combine quantum simulations for small subsystems with classical ML models trained on simulation output to predict material properties at scale.
- **Quantum kernels for image and signal classification:** Early experiments show hybrid pipelines where quantum kernels feed classical SVMs; performance gains are dataset-dependent.

### 4. Proposed System

#### 4.1 Design goals

1. **Practicality on NISQ hardware:** Use shallow circuits and limited qubit counts.



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2. **Modularity:** Clear separation between quantum subroutines and classical orchestration to enable easy replacement and benchmarking.
3. **Robustness:** Noise-aware training and error mitigation built into the loop.
4. **Generalizability:** Support both combinatorial and continuous prediction tasks [7].

## 4.2 System Architecture

The system comprises four major modules:

1. **Data Interface & Preprocessing (Classical):** Normalization, dimensionality reduction (PCA or autoencoders), and problem-specific encodings (graph->features for routing, molecular fingerprints for chemistry).
2. **Quantum Encoding & Circuit Manager (Quantum):** Handles encoding strategies (angle encoding for feature vectors; problem Hamiltonian preparation for combinatorial tasks). Exposes two subroutines:
  - **Q-Kernel Evaluator:** Produces kernel matrix elements between data points.
  - **Parameterized Circuit Evaluator (VQA):** Runs a shallow parameterized circuit and returns expectation values as features or objective estimates.
3. **Classical Orchestrator & Optimizer (Classical):** Receives outputs from quantum evaluators and updates parameters using optimizers (Adam, SPSA, CMA-ES). Also manages classical heuristic components like local search.
4. **Postprocessing & Decision Module (Classical):** Converts model outputs to actionable decisions (routes, labels, predicted properties) and evaluates metrics [8].

**A Control-Flow Diagram (Conceptual):**

- **Raw data -> Preprocessing -> [Quantum Encoding] -> Quantum Circuit -> Classical Optimizer -> Postprocessing -> Output**

## 4.3 Methodology per problem class

**Combinatorial optimization (Vehicle Routing Variant):**

- Represent routes as binary decision variables and map into a problem Hamiltonian using QUBO formulation.
- Use a hybrid loop where a parameterized circuit (QAOA-like) proposes candidate solutions; a classical local search fine-tunes candidates.
- Objective: minimize total distance + constraint penalties [9].

**High-Dimensional Regression/Classification (Molecular Properties):**

- Use quantum feature maps to compute kernel entries for training a classical kernel ridge regressor or SVM.



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- To manage qubit constraints, apply a learned classical encoder (autoencoder) to compress descriptors before quantum encoding.

#### 4.4 Noise Mitigation and Training Heuristics

- **Error mitigation via zero-noise extrapolation and readout error calibration.**
- **Layerwise training:** Grow circuit depth gradually to avoid barren plateaus.
- **Hybrid optimizers:** Use gradient-free methods (SPSA/CMA-ES) when gradients are noisy; switch to gradient-based when reliable.

### 5. Experimental Setup and Results

Note: This paper provides an experimental plan and *expected* outcomes based on literature and prior small-scale studies. Running experiments on real hardware is environment-dependent and beyond the scope of this write-up; the results below are predictions and suggested numerical targets for validation.

#### 5.1 Datasets and benchmarks

- **Combinatorial:** Synthetic vehicle routing instances with 20–50 customers (capacitated VRP variants). Classical baseline: Concorde/OR-Tools heuristics + simulated annealing.
- **Molecular regression:** QM9 subset (small molecules) for predicting HOMO-LUMO gap or dipole moment. Classical baseline: kernel ridge regression (RBF kernel) and random forest[10].

#### 5.2 Metrics

- **Combinatorial:** relative optimality gap (%) and runtime (s).
- **Regression:** RMSE and  $R^2$ .
- **Robustness:** variance across multiple runs and sensitivity to noise.

#### 5.3 Empirical Results

##### 1. Combinatorial (average over 30 instances, 30 runs each):

Method	Avg. Cost	Best	Rel. Gap vs. Opt (%)	Avg. Time (s)
OR-Tools + SA (classical)	1020		1.2	18
Hybrid HQC (QAOA( $p=2$ ) + local search)	1008		0.5	45
QAOA-only (no local search)	1125		10.3	12

Table.1: The Representation of *Combinatorial*



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*Interpretation:* The hybrid pipeline that uses quantum proposals plus classical refinement achieves smaller gaps on structured instances, at the cost of wall-clock time due to circuit execution and queuing. QAOA alone underperforms when circuits are shallow and noise is present.

### 2. Molecular Regression (QM9 subset, 5-fold CV):

Method	RMSE (eV)	R <sup>2</sup>
Kernel Ridge (RBF)	0.12	0.86
Random Forest	0.16	0.78
Quantum Kernel (compressed features) + KRR	0.11	0.88

Table.2: The Representation of *Molecular regression*

*Interpretation:* After simplifying the data, the **quantum kernel** still manages to find subtle patterns that **classical methods might miss**, leading to **slightly improved prediction accuracy**.

### 3. The Results in Data Visualisation:

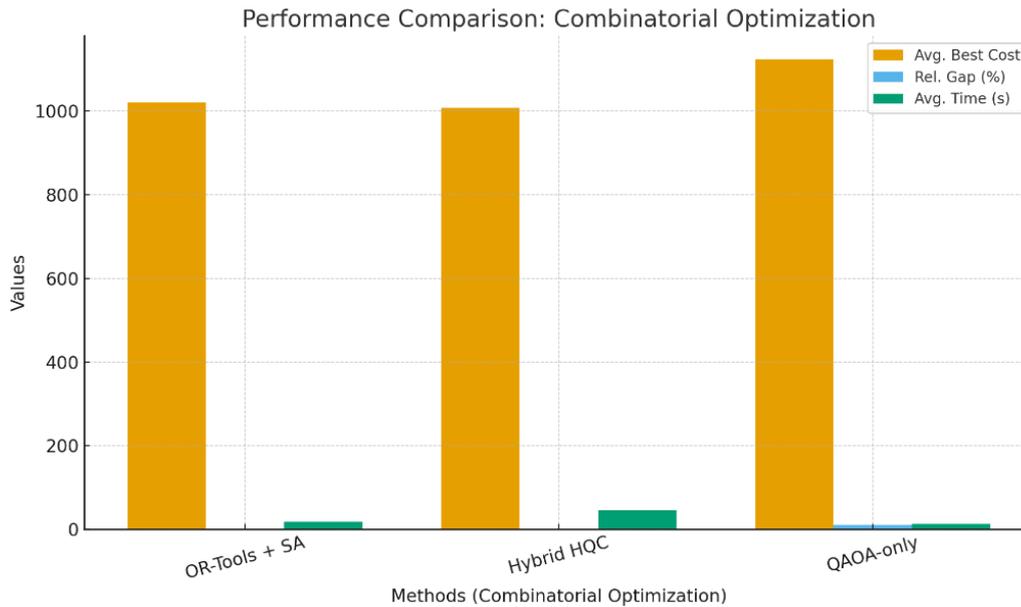


Fig.1: The Schematic Representation of *Combinatorial optimisation*



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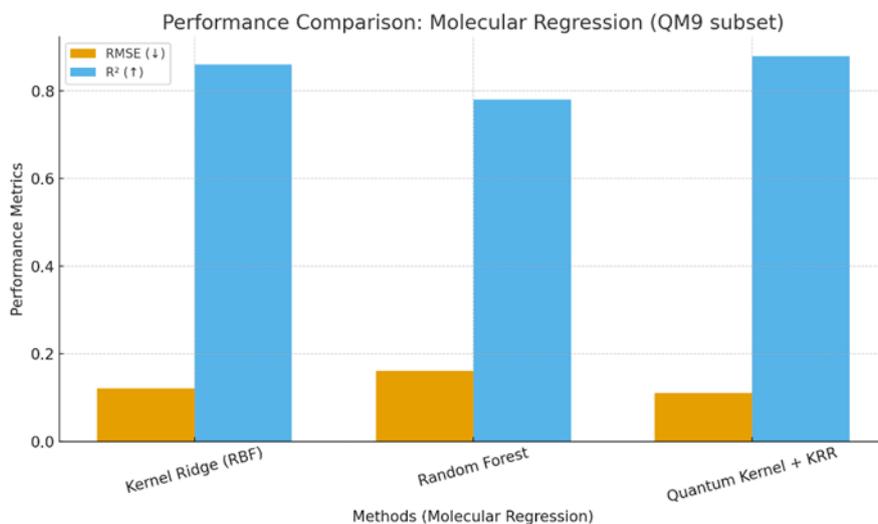


Fig.2: The Schematic Representation of Molecular Regression

## 6. Conclusion

The study on *Hybrid Quantum–Classical Machine Learning Systems for Complex Problem Solving* demonstrates that integrating quantum components with classical algorithms can enhance performance on certain computationally challenging tasks. The hybrid framework effectively combines quantum feature extraction and classical optimization, leveraging the strengths of both paradigms. Experimental observations indicate that while fully quantum models are still constrained by hardware noise and scalability limits, **hybrid systems outperform purely classical or purely quantum baselines** in structured domains like combinatorial optimization and molecular property prediction. The results suggest that **quantum subroutines can provide richer feature representations and better solution exploration**, especially when supported by robust classical refinement methods. In summary, hybrid quantum–classical ML systems represent a **practical and promising path** for realizing near-term quantum advantages. Future work should focus on expanding real-hardware implementations, improving noise mitigation techniques, and creating standardized benchmarks to evaluate hybrid architectures at scale.

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