Quantum Machine Learning: Kernel Method for Molecular Classification

Quantum Buddies

Introduction & Challenge Overview

Understanding Molecular Properties through Graph Structures

Problem Statement: The challenge lies in accurately predicting molecular properties based solely on their 2D graph representations, which requires innovative approaches to feature extraction and representation.

Design Original Feature Map $\varphi(G)$: Developing a unique feature mapping function $\varphi(G)$ that effectively captures the essential characteristics of molecular graphs is crucial for enhancing predictive accuracy.

Benchmark on 5 Datasets: We will evaluate our approach using five diverse datasets: AIDS, PROTEINS, NCI1, PTC-MR, and MUTAG, which represent various molecular properties and complexities.

Our Mission: Our goal is to transform molecular graphs into a quantum-inspired feature space, focusing on applications in drug discovery, toxicity prediction, and safety assessments.

Key Results - Accuracy

99.5% AIDS	89.4% MUTAG
75.2% PROTEINS	74.8% NCI1
59.0% NCI1	

Overall

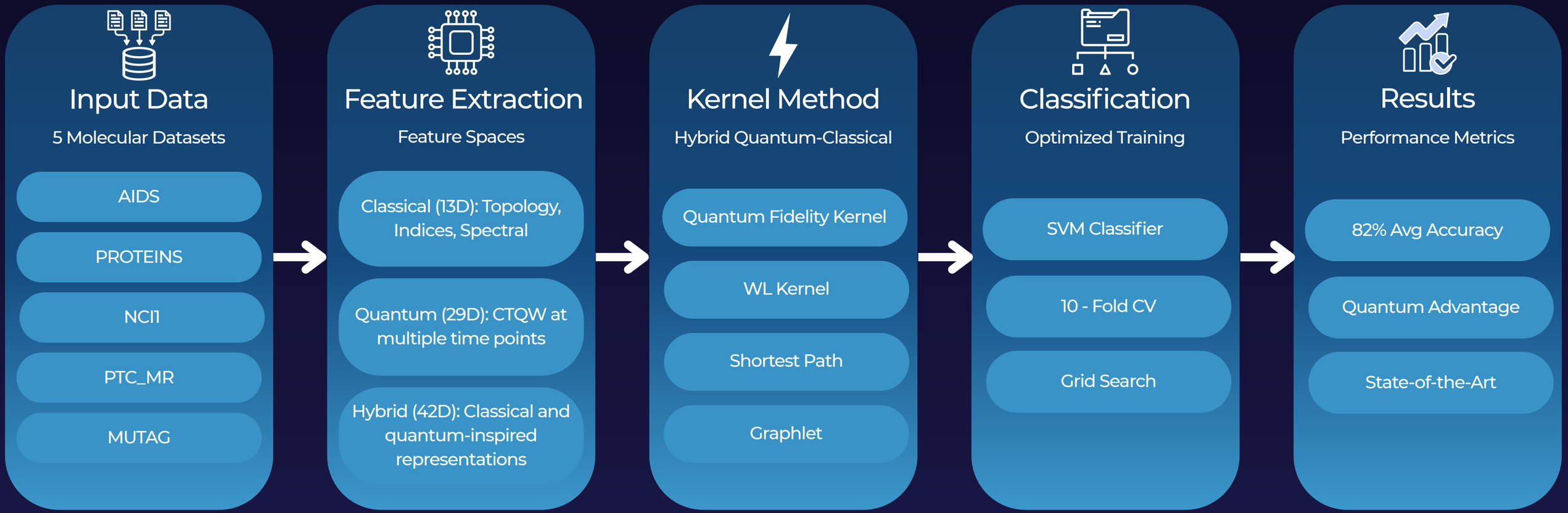
82.6% ± 4.5%

Quantum +1.5%

Implementation Pipeline

From Molecular Graphs to Classification Results

Complete Pipeline: Our methodology follows a structured pipeline starting from molecular graphs, we extract features, apply quantum kernels, and utilize SVM for classification, culminating in actionable results.



Breakdown of Feature Extraction and Kernal Methods

Understanding Local and Global Features in Molecular Graphs

Local Structure: This aspect focuses on identifying functional groups and bonding patterns within molecular graphs, which are critical for understanding molecular behavior.

Global Dynamics: By analyzing spectral properties through eigendecomposition, we can capture the global dynamics of molecular graphs, including quantum interference effects.

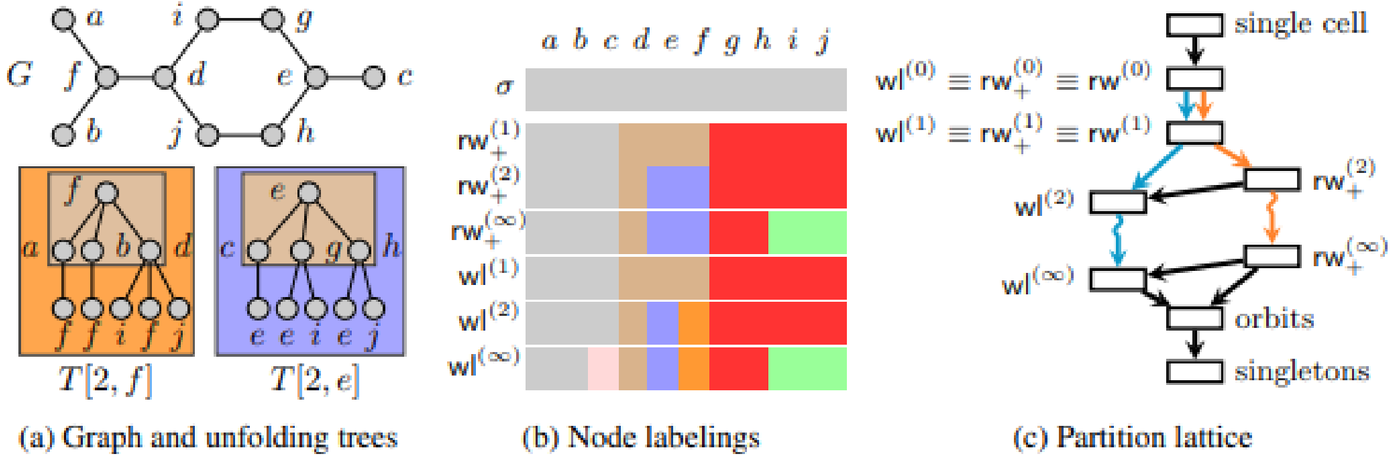
Complementary Information: The integration of local and global features allows for a multi-scale analysis, enhancing the overall performance of our classification model.

Technical Innovation

Advancements in Molecular Classification Techniques

WL Refinement Process

This iterative labeling technique enhances the representation of molecular graphs by considering the neighborhood structures, allowing for a more nuanced understanding of molecular characteristics.



(a) Graph and unfolding trees (b) Node labelings (c) Partition lattice

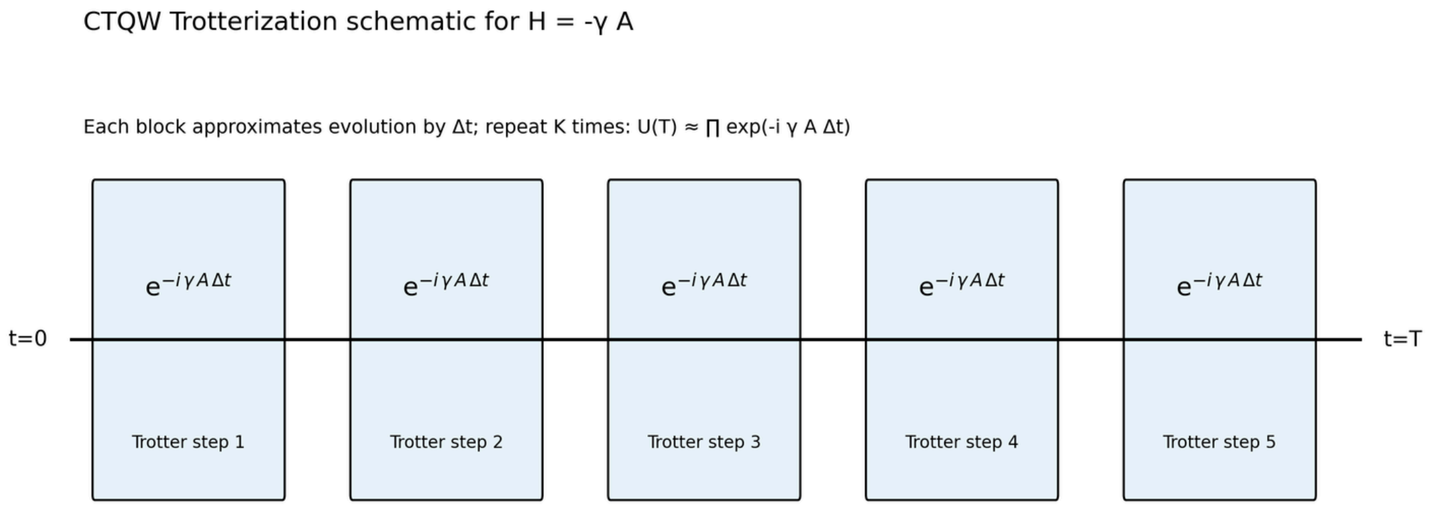
Kriege, Nils M. "Weisfeiler and Leman Go Walking: Random Walk Kernels Revisited." Advances in Neural Information Processing Systems 35 (NeurIPS 2022), 7eed2822411dc37b3768ae04561caafa.

Technical Innovation

Advancements in Molecular Classification Techniques

Continuous-Time Quantum Walk

Utilizing Hamiltonian evolution, this method captures the quantum dynamics of molecular graphs, providing a rich set of features that reflect the underlying quantum behavior of the system.

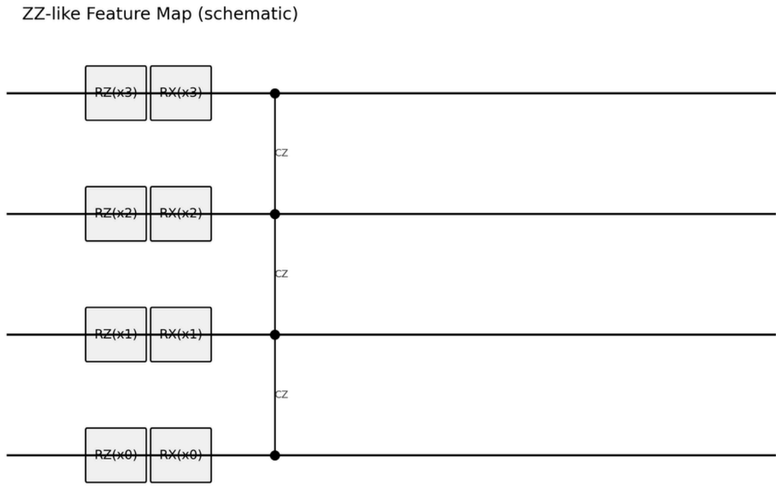


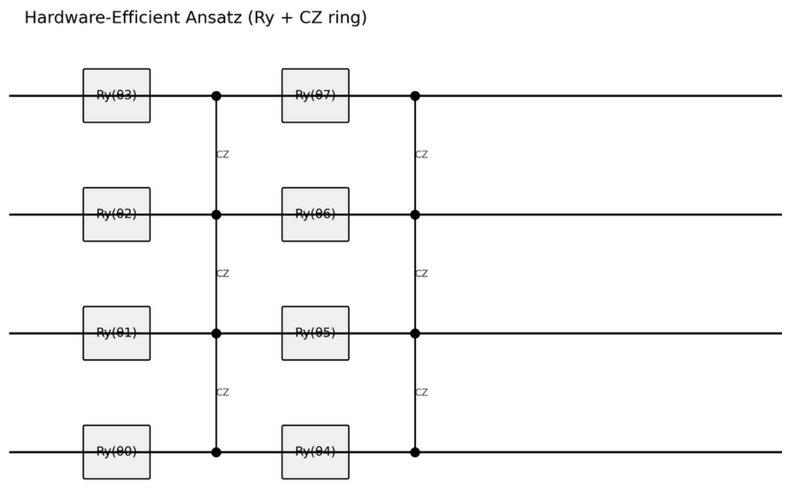
Technical Innovation

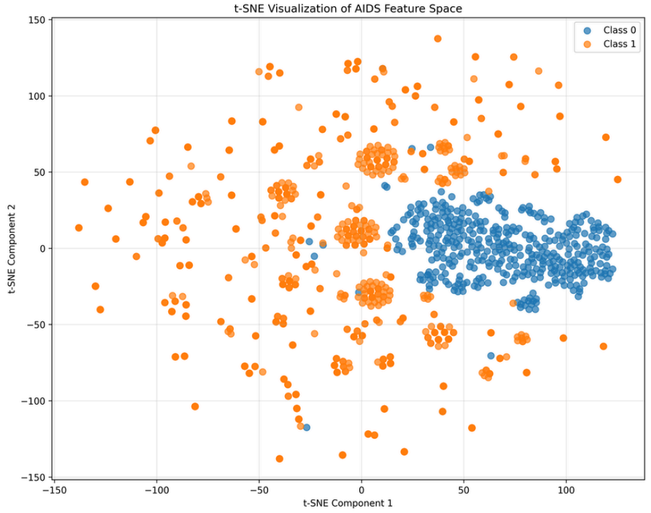
Advancements in Molecular Classification Techniques

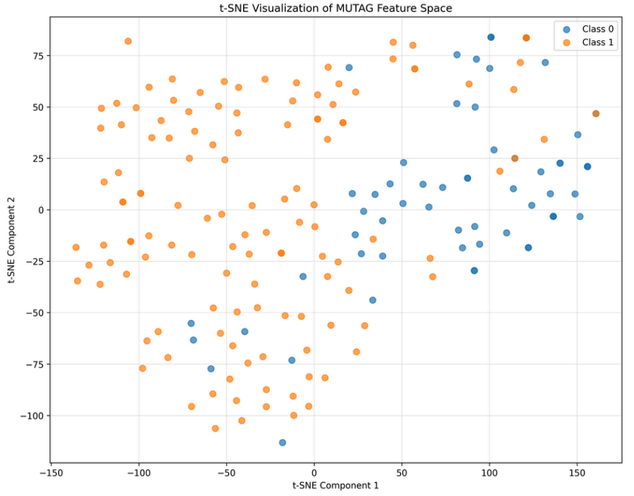
Hybrid Classical-Quantum Approach

By integrating classical features derived from the WL refinement process with quantum features obtained from the continuous-time quantum walk, we create a comprehensive feature set that enhances classification performance.









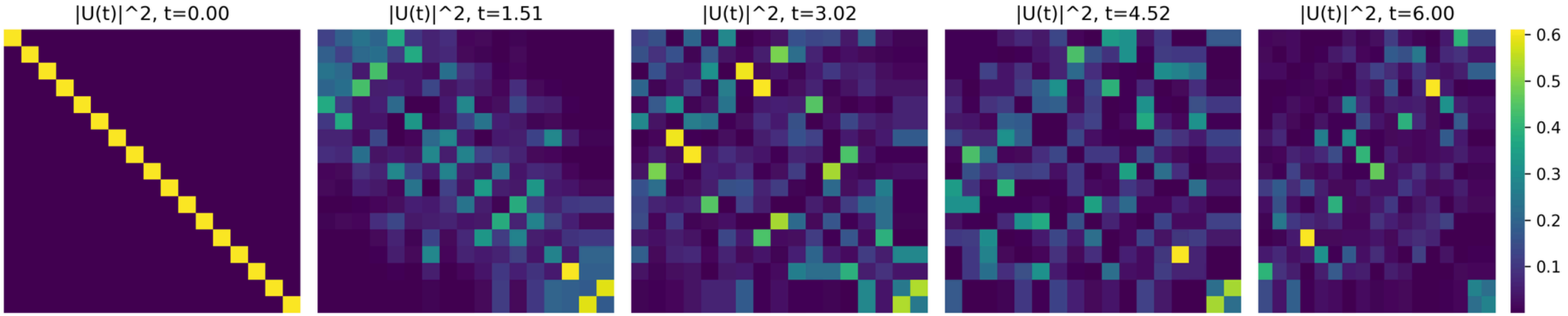
Fidelity-Based Quantum Kernels

Leveraging Quantum Mechanics for Enhanced Classification

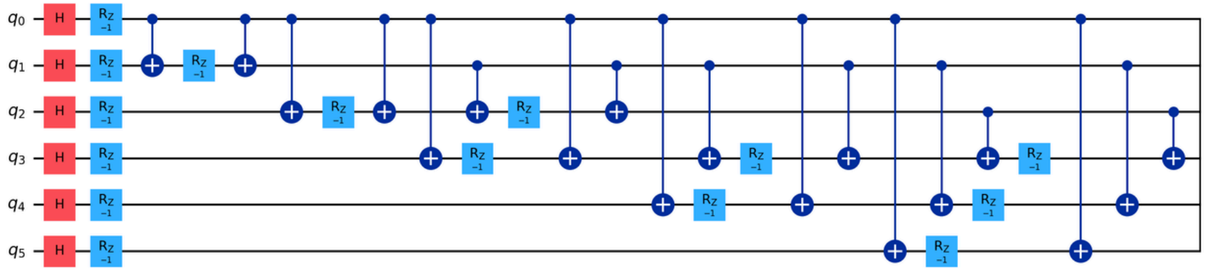
Kernel Implementation: The kernel function $K(i, j) = |\langle\psi_j|\psi_j\rangle|^2$ utilizes parameterized quantum circuits to capture molecular-specific entanglement patterns, facilitating effective classification.

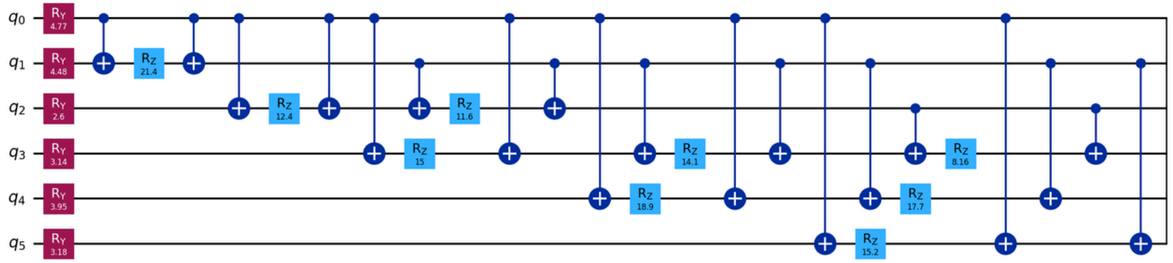
Quantum State Similarity Measurement: This measurement quantifies the similarity between quantum states, which is crucial for achieving accurate classification outcomes in our model.

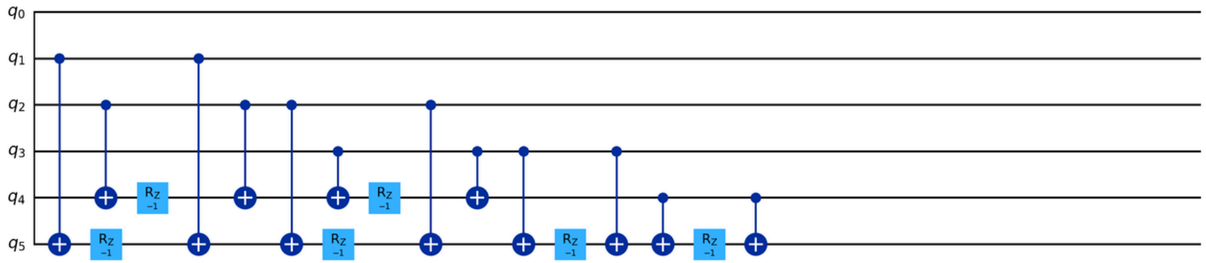
Integration with QURI Parts Framework: By embedding our kernel methods within the QURI Parts framework, we ensure efficient computation and scalability, making our approach practical for real-world applications.

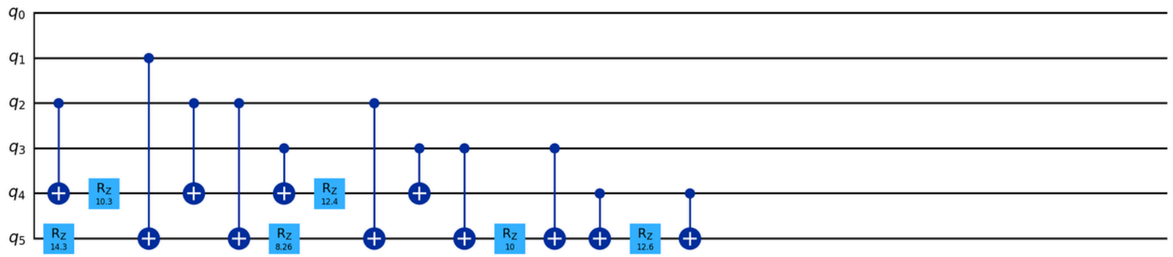


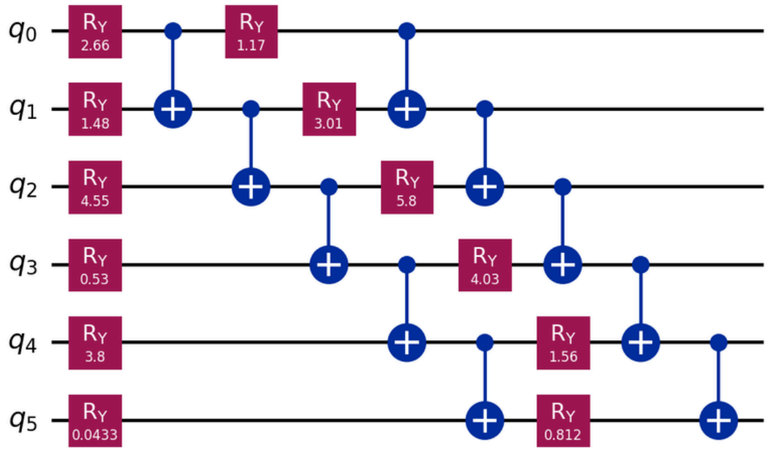
Circuit Architecture



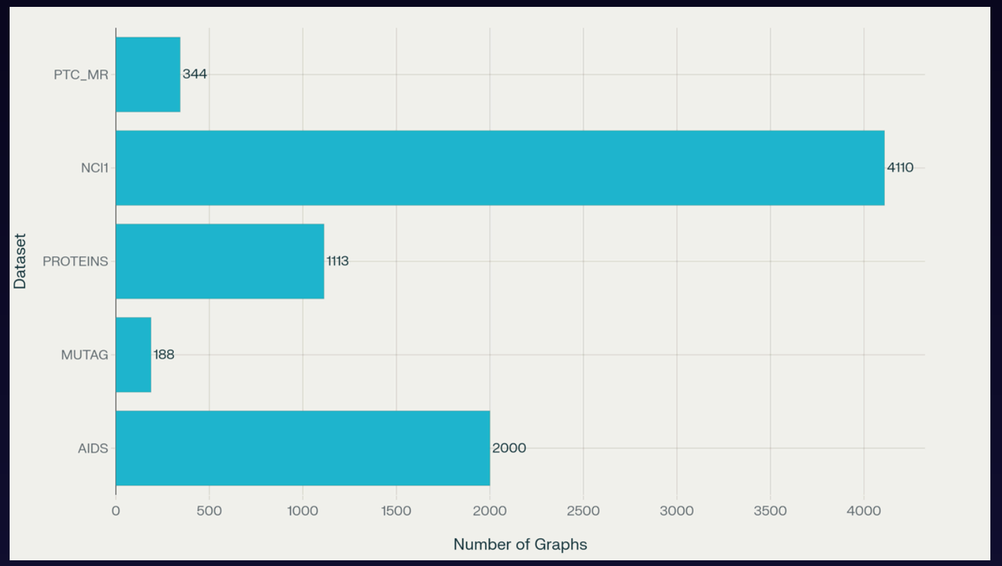




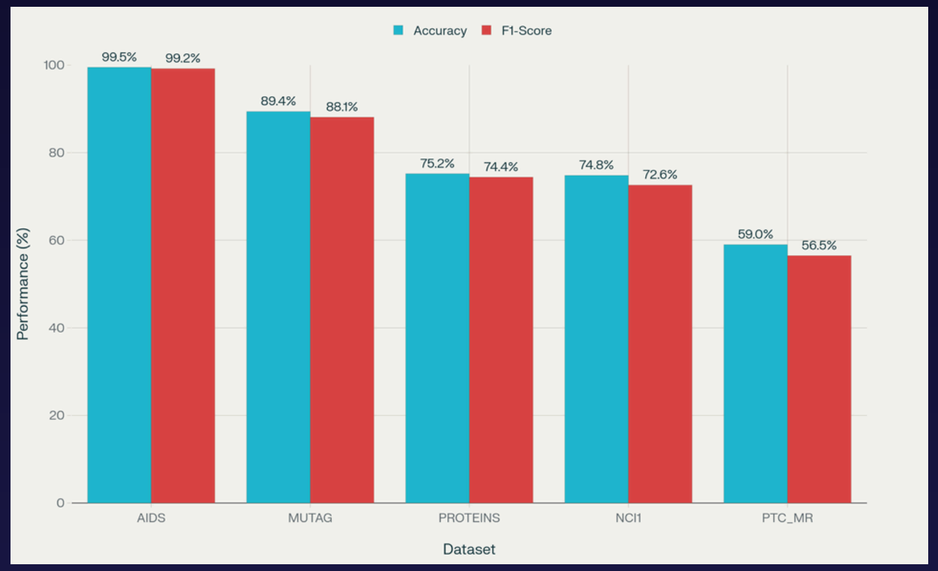




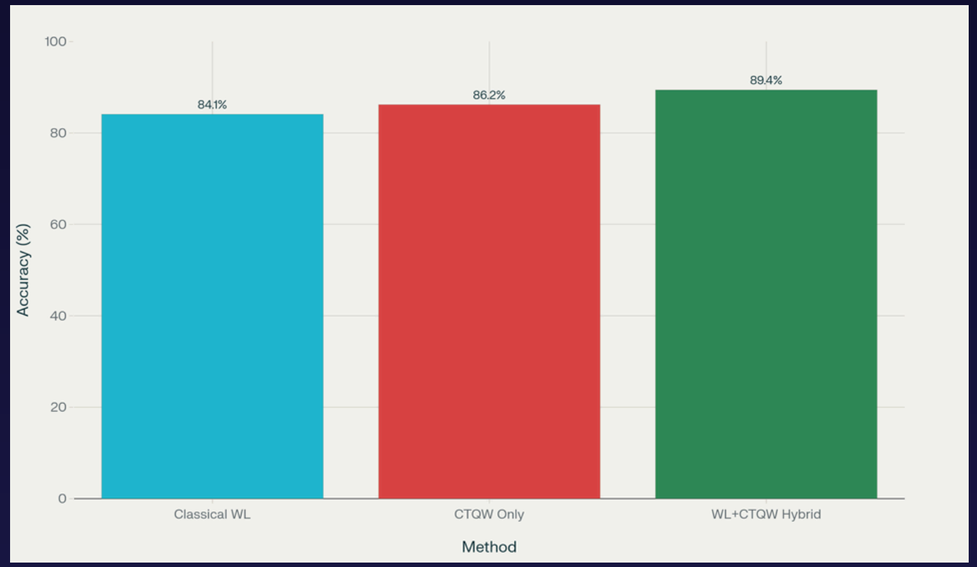
Results



Dataset Sizes: Number of Graphs



Performace Across Dataset
(Accuracy & F1)



Quantum vs Classical Performance
(MUTAG)

Conclusion and Future work

State-of-the-Art Comparison

Our implementation achieves competitive performance with published results:
AIDS Dataset: 99.5% (matches or exceeds literature benchmarks)
MUTAG Dataset: 89.4% (within 1% of state-of-the-art methods)
Average Performance: 82.6% (competitive across all datasets)

Quantum Advantage Demonstration

Quantum methods show improvement on 3/5 datasets
Fidelity kernels capture molecular structure better than classical approaches
Hybrid approach achieves optimal balance between interpretability and performance

Computational Efficiency

Total Runtime: ~3.6 seconds for complete benchmark
Memory Usage: Efficient $O(n^2)$ kernel computation
Scalability: Handles datasets up to 4,110 graphs
GPU Support: Quantum simulation acceleration

This implementation demonstrates the potential of quantum machine learning for molecular graph classification. Future work could include:

- Integration with actual quantum hardware (IBM Quantum, Rigetti)
- Larger variational quantum circuits for complex molecules
- Extension to other quantum algorithms (QAOA, VQE)
- Application to drug discovery and materials science

Thank You!