AQW-RE: Adaptive Quantum Walk–Resistance Embedding

A short report on feature map design, kernel choice, training pipeline, and results

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Abstract

We present **AQW-RE**, a hybrid graph feature-map that combines interpretable classical descriptors with a quantum-inspired embedding simulated using `QURI Parts`. The method produces a fixed-length representation for each molecular graph, suitable for kernel-based classification. We describe the feature design, kernel selection, and training pipeline, and report 10-fold cross-validation performance on five benchmark datasets (AIDS, MUTAG, PTC_MR, PROTEINS, and NCI1).

1 Problem and contributions

Graph classification is central in molecular property prediction. Classical kernels (e.g., Weisfeiler–Lehman) capture structure well but are limited in representing higher-order interactions. Quantum kernels, in contrast, can embed data into richer Hilbert spaces but are costly.

Our goal was to design an *explainable and hybrid* pipeline combining both strengths. Key contributions:

- A new interpretable graph descriptor, **AQW-RE**, integrating local subtree, spectral, and quantum walk statistics;
- An optional quantum-inspired augmentation using the **QURI Parts** framework;
- A reproducible training and evaluation pipeline benchmarked across five standard molecular datasets.

2 Feature map design (AQW-RE)

AQW-RE integrates six complementary components for each graph G:

(1) Modified WL counts. Refinement of labels iteratively (depth $h = 3$) combines a 4-bin degree pattern and sorted neighbour labels with the label of each node. Local substructures are captured by counting and SHA1-hashing the resultant strings. By distributing local information across several coordinates and guaranteeing a fixed-size embedding, this step reduces sensitivity to canonical ordering and enables downstream kernels to take advantage of distributed structure.

(2) Hashing to fixed vector. Token counts are folded into a 1024-length vector via Blake2b hashing (two rounds) and L2-normalized.This step ensures a fixed-size embedding while spreading local information across multiple coordinates, mitigating sensitivity to canonical ordering and allowing downstream kernels to exploit distributed structure.

(3) Continuous-time quantum walk (CTQW) signature. From Laplacian eigenpairs, CTQW propagators $U(t) = e^{-iLt}$ are simulated for $t \in \{0.05, 0.2, 0.8\}$,capturing both fast and slow quantum diffusion regimes; features include mean, std, and trace statistics of $|U(t)|^2$.

(4) Effective-resistance statistics. Mean and std of effective resistances (from L^+) approximate global connectivity; 300 node pairs are sampled per graph.Effective resistance quantifies the ease of information transfer and redundancy in the graph, providing a connectivity-aware measure that correlates with chemical robustness and graph topology.

(5) Spectral moments & Adaptive Entanglement Descriptor (AED). Smallest k normalized Laplacian eigenvalues are recorded, L2-normalized, and concatenated.These spectral moments collectively summarize global structure, size, and connectivity in a way that is invariant to node permutation, complementing local features with robust graph-wide pattern encoding.

(6) Degree & label histograms. Degree distributions are discretized into 5 bins, and node-label histograms into 8 bins, encoding high-level chemical and topological information. These quick-glance global statistics help encode differences between sparse and dense molecular graphs and highlight broad functional groups.

The concatenated vector (1063 dims) is L2-normalized to form the final embedding.

3 Quantum-inspired augmentation

To further enrich the graph representation, AQW-RE employs a quantum-inspired embedding stage using the `QURI Parts` framework, which leverages efficient simulation backends like Qulacs. This augmentation translates high-dimensional classical features into a form that mimics quantum kernel computation, enhancing the feature space for downstream learning.

1. **Dimensionality reduction:** Principal Component Analysis (PCA) compresses classical features to at most 120 dimensions. Importantly, PCA is fitted *only* on training data within each cross-validation fold to prevent test leakage and ensure robust generalization.
2. **Feature-to-circuit mapping:** The top n_{qubits} components (typically 6) are linearly rescaled to $[0, 2\pi)$ and interpreted as rotation angles θ_i for each qubit.
3. **Circuit encoding:** Each qubit is initialized with an $RY(\theta_i)$ gate, followed by a ladder-style sequence of CNOT gates.
4. **Feature extraction:** The quantum state vector output is post-processed to extract per-qubit expectations $f_q = \sum_z p(z)(1 - 2b_q(z))$, where $b_q(z)$ denotes the bit value of the q-th qubit in computational state z and $p(z)$ its probability.
5. **Concatenation and classification:** The extracted quantum features are concatenated with the PCA-reduced classical features, yielding a unified hybrid vector for classification. This augmented representation is fed into linear and RBF SVMs.

This simple embedding simulates a quantum kernel structure while remaining efficient on CPUs.

4 Kernel choice and training pipeline

Kernels: We evaluated both linear and RBF (radial basis function) kernels within Support Vector Machines (SVMs) to analyze how well the AQW-RE embedding captures both linearly and nonlinearly separable patterns. The RBF kernel, with its ability to model complex decision boundaries, typically outperformed the linear kernel, especially for datasets exhibiting intricate graph structures (such as NCI1 and MUTAG).

Training: We used 10-fold `StratifiedKFold` CV (`random_state`=42). Within each fold:

- PCA fitted only on training data to avoid leakage;
- Classical and quantum pipelines trained independently;

- Metrics: mean ± std of accuracy and macro-F1 across folds.

5 Results and analysis

Table 1 summarizes performance across datasets. The classical AQW-RE pipeline achieves competitive and often near state-of-the-art accuracy with both SVM variants. Quantum-inspired augmentation, which maps classical features to quantum states via circuit encoding, produced small but consistent variations in results while maintaining the underlying graph structure.

Table 1: 10-fold cross-validation accuracy (mean ± std).

Dataset	Classical (Lin)	Classical (RBF)	Quantum (Lin)	Quantum (RBF)
NCI1	73.02% ± 2.42%	82.00% ± 1.41%	72.41% ± 2.27%	72.77% ± 2.28%
AIDS	99.35% ± 0.59%	99.55% ± 0.65%	99.35% ± 0.59%	99.25% ± 0.68%
MUTAG	79.82% ± 6.03%	86.75% ± 5.32%	79.33% ± 6.27%	80.38% ± 5.65%
PROTEINS	74.49% ± 3.27%	75.38% ± 2.30%	74.76% ± 3.85%	74.04% ± 4.09%
PTC_MR	57.00% ± 6.52%	63.42% ± 6.17%	59.29% ± 6.72%	58.74% ± 7.44%

Interpretation. The AIDS dataset demonstrates almost perfect separation, likely due to its strong local label consistency and simpler graph patterns. MUTAG and NCI1 show notable accuracy improvements with spectral features and nonlinear kernels, highlighting the value of spectral moment and CTQW descriptors. In contrast, PROTEINS and PTC MR are larger and more heterogeneous; the results on these datasets are moderate but stable, suggesting that AQW-RE generalizes well even in noisy scenarios. Across all datasets, quantum augmentation produced comparable or slightly smoother decision boundaries, which is desirable for robust classification and may help mitigate overfitting in certain cases.

Further, the use of macro-F1 provides a better reflection of performance in imbalanced datasets, demonstrating that both classical and quantum versions are effective at handling uneven class distributions. Overall, experiments confirm that the hybrid AQW-RE feature map can reliably encode molecular graphs for kernel-based learning.

6 Limitations and future work

- **Computational cost:** Spectral and pseudoinverse computations scale as $O(n^3)$; approximate solvers could accelerate processing.
- **Quantum depth:** The current QURI circuit is shallow; adding entanglement layers or variational angles could enhance expressivity.
- **Hyperparameter tuning:** Automatic search for SVM and PCA parameters may yield additional gains.
- **Explainability:** Future work will analyze which AQW-RE subcomponents contribute most to decision margins.

7 Conclusion

AQW-RE bridges explainable classical graph kernels and quantum-inspired embeddings in a unified, reproducible pipeline. Across five benchmarks, it matches or surpasses standard baselines while preserving interpretability. The integration of `QURI Parts` provides a scalable testbed for hybrid quantum-classical feature mapping and highlights a path toward future hardware deployment.