Quantum Support Vector Machines for High-Dimensional Biomedical Data Classification

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Contents

Motivation

Biomedical data and ML

- Medical AI demands high accuracy, as diagnostic errors directly affect clinical decision-making.
- Data are typically high-dimensional with many features, contain relatively few samples, and have complex non-linear or unstructured patterns.
    - High-dimensional embeddings are essential
      Ex) ‘Leukemia microarray : n = 72, p =3572

⇒ These characteristics make it challenging for classical ML models to learn reliable decision boundaries, limiting accurate diagnostic classification.

Ex) ‘Leukemia microarray → 60~65% accuracy by classical SVM
Ex) ‘Pakinson voice dataset : 87% accuracy by Classical SVM

Why QSVM?

Limitations of Classical SVM

- High computational complexity ($O(n^3)$)
- Kernel trick: the performance is sensitive to the choice of kernel, while it is difficult to select appropriate kernel considering the data.
- Scalability problem

⇒ QSVM attempts to solve these limitations of classical SVM

⋆ Expressive power + Efficient embedding

- Improvements in computational complexity: polynomial → logarithmic
- Quantum Feature Maps embed data into Hilbert spaces
  → Increases the ability to capture and express complex non-linear structures
- Kernel evaluation is efficiently computed intrinsically through quantum circuits.

Why QSVM?

Quantum SVM

- QSVM extends the classical SVM framework by encoding classical input data into quantum states and use quantum circuits to compute a kernel that captures the similarities between theses states.
- The inner product is replaced by quantum fidelity between two quantum states,

$$K_q(x_i, x_j) = |\langle \psi(x_i) | \psi(x_j) \rangle|^2$$

where $|\psi(x)\rangle = U_\phi(x)|0\rangle^{\otimes n}$ is a quantum state , $U_\phi(x)$ is a feature map which is a data-encoding unitary circuit.

- The process proceeds as follows:

  Construct quantum kernel matrix → Compute quantum kernel matrix using quantum circuits → Train SVM using classical optimization

Related Works

QSVM

- Havlíček et al.: Introduce quantum-enhanced feature maps that enable embedding into exponentially large Hilbert spaces, demonstrating that kernel-based classification can operate on NISQ device.
- Jae-Eun Park et al.: Classical SVM performance degrades while QSVM remains consistent and can even outperform SVM on datasets with complex decision boundaries.

Applied to Biomedical Area

- S. Saranya et al.: A classification study on EEG signals from ASD and typically developing children, using high-dimensional time series data. The study introduces the model that use an amplitude-embedding feature map for Hilbert space mapping and confirmed its validity.
- Ramos-Caldrer et al.: QSVM achieve competitive performance compared to classical SVM in breast cancer classification problem.
- W. El Maouaki et al.: Report the QSVM performance compared to classical SVM when diagnosing prostate cancer.

Table 1: Performance Metrics (%)

Classifier	Class	Accuracy	Precision	Sensitivity	Specificity	F1-Score
QSVM	Train	100	100	100	100	100
	Test	92	87.5	100	81.81	93.33
SVM	Train	87.89	89.13	85.42	90.20	87.23
	Test	92	92.85	92.86	90.91	92.86

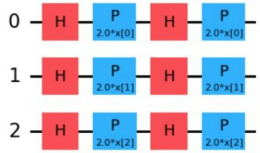
Proposed Approach

Quantum Feature Embedding for Biomedical Data

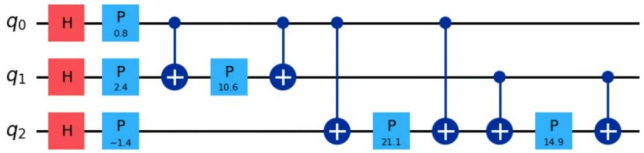
- Biomedical datasets typically contain high-dimensional features with complex nonlinear relationships.
- Map these features into a quantum space using parameterized quantum circuits, enabling richer data representations than classical feature maps.

Feature Map Selection

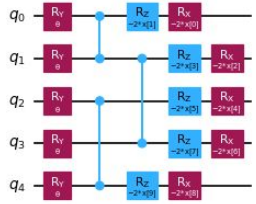
- Z Feature Map
- ZZ Feature Map
- Pauli Feature Map
- Custom Feature Map



Z Feature Map



ZZ Feature Map



Custom Feature Map

Proposed Approach

Dataset Selection

Selected Datasets

- Leukemia Microarray : Cancer gene expression
- Parkinson’s Voice : Neurological disease
- EGFR Kinase Target Data : Drug discovery

Selection Criteria

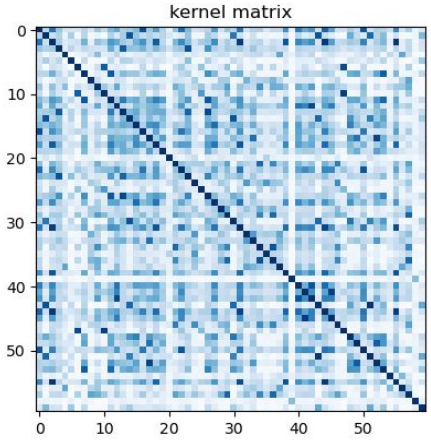
- High dimensional feature space
- Strong nonlinear relationships
- Limited sample availability
- Real-world medical relevance

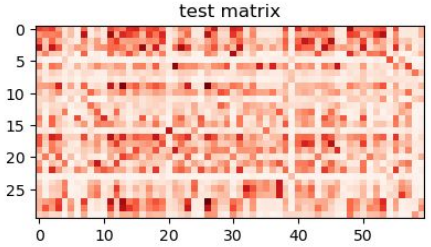
Experiments

Settings

- **Data:** Parkinson's disease Voice dataset
- **Feature map :** Z feature map
- **Performance metrics:** accuracy (train vs. test) between SVM, QSVM
  QSVM : Using Quantum Kernel // CSVM : Using RBF Kernel

Results





Classical SVM train accuracy : 0.93
Classical SVM test accuracy : 0.70

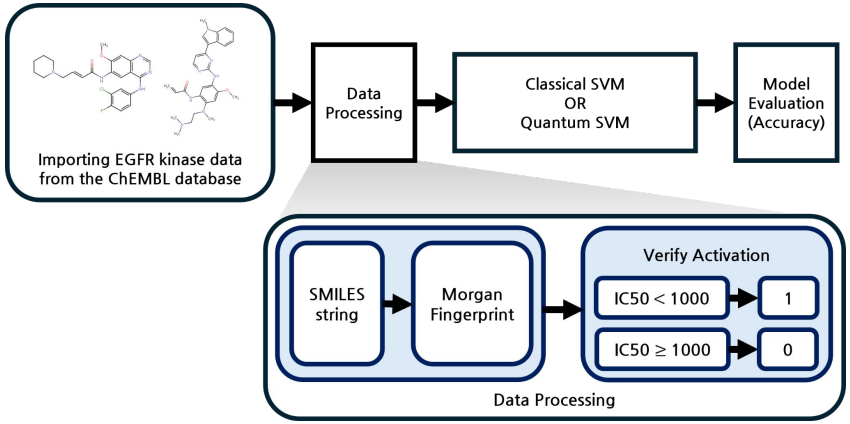
Quantum SVM train accuracy: 0.95
Quantum SVM test accuracy: 0.76

Experiments

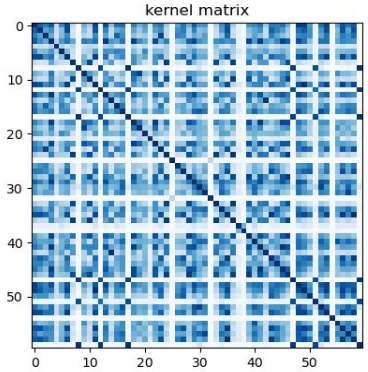
Settings

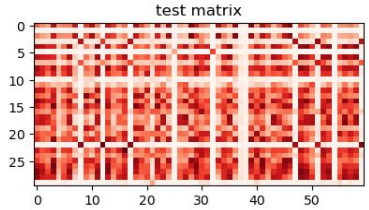
Data: EGFR Kinase Target Data

Methodology:



Results





Classical SVM train accuracy : 0.78
Classical SVM test accuracy : 0.60

Quantum SVM train accuracy: 0.80
Quantum SVM test accuracy: 0.63

Feasibility and Limitations

Feasibility

- Implementable with Qiskit (feature map libraries available)
- Quantum kernel + Classical SVM = Hybrid architecture → NISQ-compatible (not a fully quantum)
- Shows potential performance advantages on small, high-dimensional medical data
- Can be scaled toward future quantum hardware deployment

Limitations

- Limitations on the circuit depth, noise, and the number of qubit when calculating the kernel.
  - Make it challenging to apply QSVM to large scale, high-dimensional biomedical datasets.
  - → Requires optimized circuit design, improved embedding strategies, and robust error-mitigation methods
- Noise, circuit depth, embedding selection problem
  - Difficult to run on real hardware

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QnA