IMPLEMENTATION OF A HYBRID QUANTUM-CLASSICAL SYSTEM FOR DRUG DISCOVERY

DESCRIPTION

Provide a comprehensive overview of your project, including:

OBJECTIVE:

Develop a hybrid quantum-classical system that enhances drug-target interaction (DTI) prediction by leveraging quantum feature selection (QAOA/VQE) and classical machine learning (Neural Networks, SVM, Random Forest).

BACKGROUND:

Predicting DTI is crucial for drug discovery, helping to identify potential drug candidates efficiently. Traditional methods rely on computationally expensive feature selection techniques. Quantum computing, particularly QAOA and VQE, offers a promising alternative by optimizing molecular feature selection, potentially improving accuracy and computational efficiency.

TECHNICAL APPROACH:

1. Data Preparation

- Dataset Acquisition: Use publicly available datasets such as PDBbind or DrugBank, containing molecular descriptors and binding affinities.
- Data Preprocessing: Handle missing values, normalize numerical features, and encode categorical variables.
- Feature Extraction: Represent molecular structures numerically using descriptors like ECFP (Extended Connectivity Fingerprints) or Mordred descriptors.

2. Quantum Feature Selection (QAOA/VQE)

Problem Formulation: Define feature selection as an optimization problem using a cost Hamiltonian:

$$H_c = \sum_{ij} w_{ij} z_i z_j + \sum_i b_i z_i$$

- Ansatz Selection: Use a parameterized quantum circuit for QAOA or VQE to optimize feature selection.
- Quantum Circuit Construction: Implement circuits in any platforms, optimizing CX-gate count and circuit depth for efficient execution.

3. Hybrid Model Integration

- **Classical-Quantum Hybrid Model:**
    - Use QAOA/VQE-selected features to train classical ML models like Neural Networks, Random Forest, or SVM.
    - Compare quantum-selected features against traditional methods like PCA and LASSO.
- **Training and Optimization:**
    - Optimize parameters using gradient descent (classical) or quantum gradient techniques (QAOA/VQE optimizers).

4. Model Evaluation and Validation

- Performance Metrics: Measure accuracy, precision, recall and F1-score to evaluate predictive capability.
- Benchmarking: Compare quantum-enhanced feature selection against classical methods in terms of prediction accuracy, feature selection efficiency, and computational complexity.

References:

- J. K. Lim, D. G. Dickson, J. A. Black et al., "Hybrid Quantum-Classical System for Drug Discovery," *National Library of Medicine*, vol. 13, no. 8, pp. 1-10, Aug. 2022. https://pmc.ncbi.nlm.nih.gov/articles/PMC9333455/.
- Perdomo-Ortiz, N. Dickson, M. Drew-Brook, G. Rose, and A. Aspuru-Guzik, "Finding low-energy conformations of lattice protein models by quantum annealing," *Phys. Rev. Lett.*, vol. 111, no. 13, pp. 130505, Sep. 2013.
- K. S. Kumar, S. S. S. R. Depuru, and S. Arumugam, "Drug Target Interaction Prediction Using Variational Quantum Classifier," *2022 IEEE International Conference on Quantum Computing and Engineering (QCE)*, Broomfield, CO, USA, 2022, pp. 1-8.

This implementation explores the practical application of quantum computing in drug discovery by integrating quantum feature selection techniques with classical machine learning models. By leveraging algorithms like QAOA or VQE, the study aims to enhance the selection of molecular descriptors, optimizing drug-target interaction predictions. The project will compare quantum-based feature selection with classical methods such as PCA, RFE, and mutual information-based selection, evaluating efficiency, accuracy, and computational complexity.

A key focus is benchmarking quantum and classical approaches based on feature selection efficiency, prediction accuracy, circuit depth, and CX-gate count. This comparative study will assess whether quantum computing provides a significant advantage in processing complex biochemical data. The findings will contribute to understanding quantum computing's potential in drug discovery and its role in improving predictive modelling for drug repurposing.