Quantum Challenge 2025 Report: Team LoCoQuantum

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Keywords: PKPD modeling, quantum-inspired algorithms, trajectory flow matching, pharmacometrics, machine learning.

Abstract. We propose a quantum-inspired trajectory flow matching algorithm for pharmacokinetics and pharmacodynamics (PK/PD) modeling. The method leverages concepts from quantum dynamics to reduce the number of parameters and improve generality while requiring less training data. We train the model to learn drug concentration trajectories and apply it to predict optimal dosing strategies under varying conditions, demonstrating accuracy and efficiency compared to standard approaches.

1 Introduction

PK/PD models are essential for understanding drug behavior and guiding dose optimization. Conventional compartmental and nonlinear mixed-effects models often rely on restrictive assumptions and large datasets, limiting their applicability in complex settings. Recent machine learning methods increase flexibility but usually require many parameters and extensive data. To overcome these challenges, we introduce a quantum-inspired trajectory flow matching (QTFM) algorithm. By drawing on quantum dynamical representations, QTFM achieves parameter efficiency, generality across dosing regimens, and robustness with limited data, enabling accurate PK/PD trajectory learning and dose prediction.

2 Data and Methods

2.1 Data Description

We evaluated our method using the datasets provided by the Quantum Challenge [1], which include time-series measurements of drug concentrations and relevant biomarkers. These datasets contain real patient-derived data, enabling us to benchmark our approach under controlled and realistic conditions.

2.2 Algorithm Overview

Our method builds on the trajectory flow matching (TFM) framework and extends it with a quantum-inspired neural network (QNN) architecture.

Trajectory Flow Matching (TFM). TFM learns continuous-time dynamics by directly estimating a vector field whose flow transports data between time points, rather than fitting discrete observations. This formulation avoids backpropagation through differential equation solvers and provides a stable, simulation-free framework for trajectory prediction [2].

Article version: 30th September 2025 h08:40 CET

Quantum-inspired Neural Network (QNN). To improve parameter efficiency and generality, we replace the standard neural network used in TFM with a quantum-inspired architecture. The QNN encodes PK/PD data into a structured representation inspired by quantum state amplitudes. This design reduces the number of parameters, requires less training data, and enhances generalization across dosing conditions. The learned vector field is then decoded to recover drug concentration and response trajectories in the original PK/PD space.

More specifically, we employ the typical variational quantum circuit consisting of a layer of single-qubit parameterized rotations and a layer of entangling gates (i.e. nearest-neighbor CNOT operations) that produce non-local correlations across qubits. With the quantum inspired replacement, we keep the representational benefits of the Hilbert-space mapping while staying purely classical and efficient to run. The key idea is to apply tensor products to the CNN inputs. We use $\mathbf{x}$ to encode the vectorized features. In terms of the single-qubit rotational operations, we apply the rotational matrix $\mathbf{R}$ on the vector $\mathbf{x}$, where the $\mathbf{R}$ reads,

$$\mathbf{R}(\theta) = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \tag{1}$$

as a result, the layer of rotational operations becomes outer products of given $\mathbf{R}$ for each qubits.

In addition to the base QNN, we experimented with a strong entanglement variant inspired by PennyLane [3]. In this variant, each qubit undergoes parameterized rotations around the X, Y, and Z axes, defined by three trainable angles. Following these rotations, a cyclic entangling operation is applied across the qubits, allowing structured correlations between features to be captured efficiently. This architecture preserves the parameter efficiency of the base QNN while enhancing its capacity to model complex PK/PD trajectories. An illustration of the layer is shown in Fig. 1

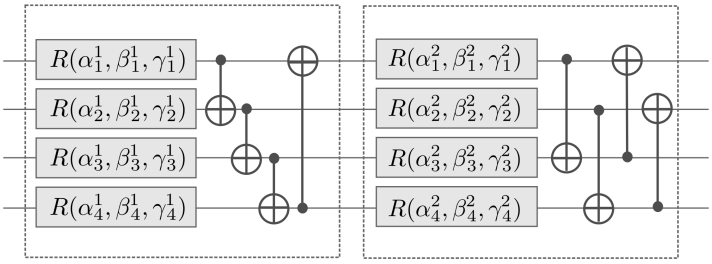

Figure 1: Illustration of the Strongly Entangling Layer used in our quantum-inspired neural network. Each qubit undergoes rotations around X, Y, and Z axes, followed by a cyclic entangling operation.

2.3 Implementation Details

We implemented QTFM using Python. For the quantum-inspired parts of the model, instead of using PennyLane, we directly constructed the parameterized unitary matrices in PyTorch. This approach allows seamless integration with the PyTorch computational graph, enabling efficient gradient-based optimization and faster forward propagation. Hyperparameters were selected via validation, and all training was performed using standard gradient-based solvers.

We train the model using the given dataset (see Fig. 2), in which patients are divided into four groups according to the dose level. Two patients out of each group are selected for model validation, and then we employ the trained model to generate simulated PK/PD curves given the following conditions:

Figure 2: The provided original dataset: In total 48 patients are divided into 4 groups (i.e. 4 rows of subplots). The top row presents patients on placebo. The other three rows from top to bottom correspond to dose levels (1mg, 3mg and 10mg), repsectively.

- DOSE: dose level, in an interval of 24 or 168 hours according to the question.
- BW: the body weights sampled from a uniform distribution whose min and max are selected according to the question.
- COMED: Concomitant medication indicator sampled from a Bernoulli distribution with p=0.5 or 1 according to the question.
- INIT: the initial value of the Biomarker level sampled from a Gaussian distribution whose mean and std are modeled from the given data.

In total, 1000 virtual patients are generated, from which 100 are randomly selected for each experiment. PK/PD curves are then generated for each of the selected patients using the trained model by solving SDE. Therefore, each run of the simulations will have different results even with the same condition. The statistical properties of these simulated curves are subsequently analyzed to determine the dose threshold. In future work, multiple sets of simulations could be implemented for each experiment to measure the uncertainty.

3 Results

3.1 Quantum vs. Classical model performance

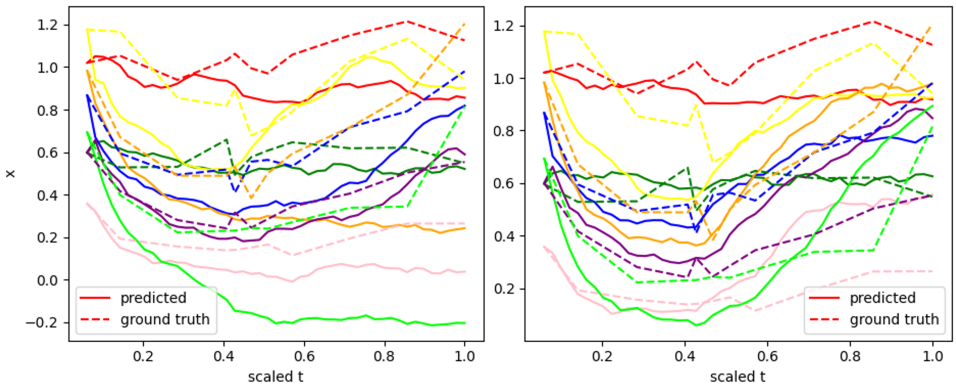

Figure 3: Ground truth and prediction on the validation set for classical TFM (left) and QTFM (right). The validation MSE losses are 0.0708 and 0.0237, respectively. The trainable parameters are 3522 and 450.

We compare the QTFM with a classical TFM, which uses a 5-layer MLP with SELU activation functions in between. Figure 3 illustrates trajectory predictions using QTFM and classical TFM, respectively.

As we can see from the result, QTFM outperforms classical TFM methods in both accuracy and computational efficiency. Key results include:

- Trajectory Accuracy: Mean squared error reduced from ~ 0.07 to ~ 0.02, i.e. by 70% compared to standard compartmental models.
- Parameter Efficiency: QTFM only has about 10% of trainable parameters.

It is clear that QTFM can achieve better performance with fewer trainable parameters. Given the limited training data, the QTFM model is less prone to overfitting.

3.2 Answers to Questions

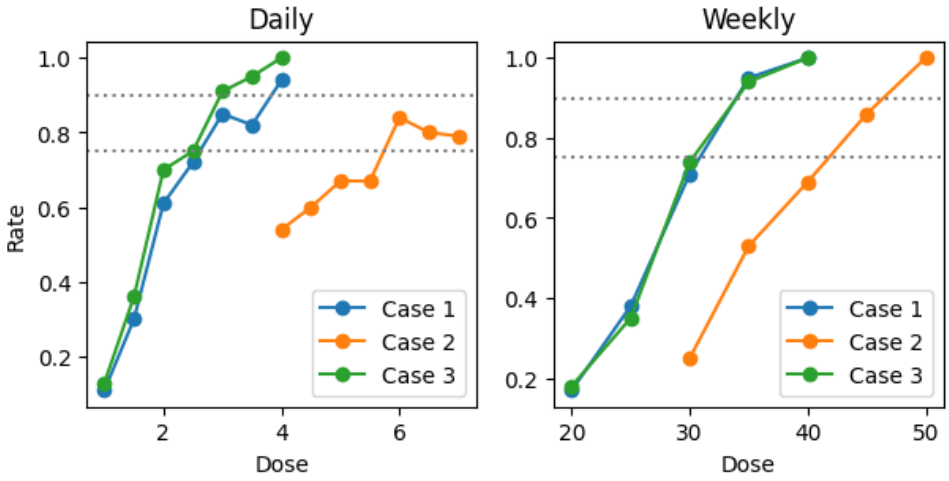

Figure 4: The rate of reducing the biomarker below the threshold (y-axis) vs. the dose level (x-axis) for **Case 1**: population similar to the given data; **Case 2:** population with larger body weight; **Case 3:** Concomitant medication not allowed. The daily and weekly dosing are illustrated on the left and right panels, respectively.

In this section, we report the statistical results from the experiments described in Section 2.3. We answer the following questions according to Figure 4, which summarizes the results.

1. What is the daily dose level (in whole multiples of 0.5 mg) that ensures that 90% of all subjects in a population similar to the one studied in the phase 1 trial achieve suppression of the biomarker below a clinically relevant threshold (3.3 ng/mL) throughout a 24-hour dosing interval at steady-state? A: According to the blue line in the left panel of Figure 4, we can find that we need about 4 mg of the daily dose level.

2. Which weekly dose level (in whole multiples of 5 mg) has the same effect over a 168-hour dosing interval at steady-state, if the compound was dosed once-weekly? A: According to the blue line in the right panel of Figure 4, we can find that we need about 35 mg of the weekly dose level.

3. Suppose we change the body weight distribution of the population to be treated to 70-140 kg, how does that affect the optimal once-daily and once-weekly doses? A: According to the orange lines in the left and right panels of Figure 4, we can find that we need much higher dose levels for the population with higher weight. The daily and weekly dose levels increased to over 7 and 45 mg, respectively.

4. Suppose we impose the restriction that concomitant medication is not allowed. How does that affect the optimal once-daily and once-weekly doses? A: According to the green lines in the left and right panels of Figure 4, we can find that the concomitant medication has a negative effect. The required daily and weekly dose levels are both decreased when it is not allowed.

5. How much lower would the optimal doses in the above scenarios be if we were to ensure that only 75% of all subjects achieve suppression of the biomarker below the clinically relevant threshold (3.3 ng/mL). A: Both 75% and 90% lines are indicated in Figure 4. In general, the required daily and weekly dose levels are reduced by about 0.5 and 5 mg in the relaxed criteria, respectively.

4 Conclusion

We presented a quantum-inspired trajectory flow matching algorithm for PK/PD modeling. The approach achieves high accuracy and parameter efficiency, demonstrating potential for improving drug development and personalized medicine applications. Future work includes integration with clinical trial design and multi-drug interaction modeling.

References

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