Quantum Challenge 2025: Team Qitchen

Brief Information for Challenge

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Quantum machine learning offers promising work for humanity in the healthcare sector, demonstrating its significant potential. Therefore, this study aimed to perform prediction using variational quantum neural networks, a type of quantum machine learning. To this end, different coding techniques were tested to determine the best prediction. In this process, calculations were performed using amplitude and angle encoding in the Pennylane library. Based on the results, amplitude encoding, by reducing the dataset, yielded better R^2, MAE, MSE scores than both angle encoding and feature-reduced angle encoding. In addition, it has been shown that very close results are obtained in the scores when the feature-reduced angle embedding.

Angle Embedding
```
MAE: 1.7569571733474731
MSE: 6.876602649688721
R^2: 0.47979438304901123
Std of preds: 2.9132302
```

Reduced-Feature Angle Embedding
```
Best Test MAE: 1.7572272552391448
Best Test MSE: 7.015986575060025
Best Test R^2: 0.46925014165709367
```

Reduced Data Amplitude Embedding
```
Best Test MAE: 1.612947630521802
Best Test MSE: 5.661935281993452
Best Test R^2: 0.5716822834942471
```

References:

Kocabay, Samet, et al. "Prediction of newly synthesized heparin mimic’s effects as heparanase inhibitor in cancer treatments via variational quantum neural networks." Computational Biology and Chemistry 118 (2025): 108476.

Ville Bergholm et al. *PennyLane: Automatic differentiation of hybrid quantum-classical computations.* 2018. arXiv:1811.04968