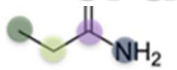
Quantum Machine Learning
Improving Binding Affinity Predictions for Drug Discovery

Sambit Banerjee, Shawn He Yuxun, Shiva Konakanchi, Lawal A. Ogunfowora, Shaswata Roy, Suriya Selvarajan, Gauri Vaidya (TA)
Corporate Partners Mentors: Laia Domingo Colomer, Marko Djukic, Christine Johnson

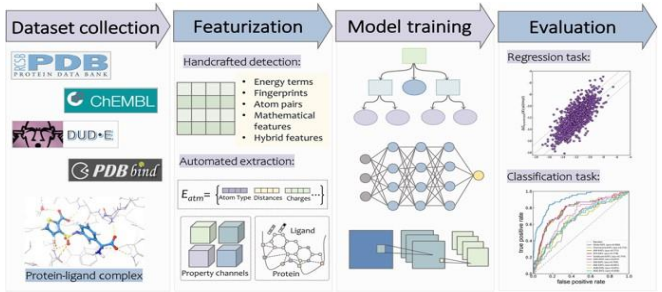
Scan this QR code for access to our paper

The Heart of the matter



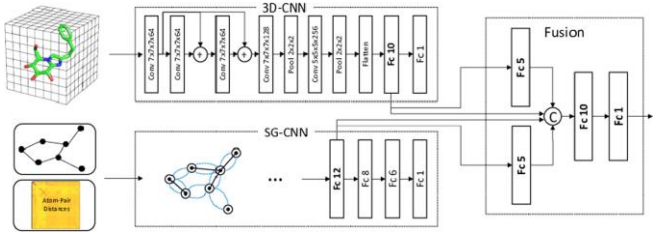
To identify suitable drug candidate compounds, ML/DL has been used to predict binding affinities between small chemical compounds (i.e. ligands) and proteins---thereby greatly reducing the time, labor and costs otherwise involved in measuring it *experimentally*. We use the state-of-the-art classical algorithm for such predictions using a fusion of a 3D Convolutional Neural Network (3D-CNN) and a Spatial Graph Convolutional Neural Network (SGCNN) and replace the fusion layers with a feed-forward quantum neural network, thereby obtaining improved predictions.

1. The Grand Scheme

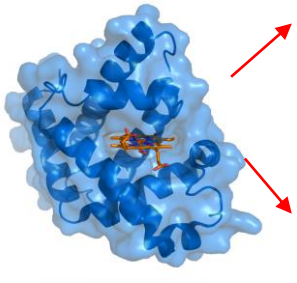


Workflow for ML prediction of protein-ligand binding affinity [1]

2. The Classical State-of-the-art Model

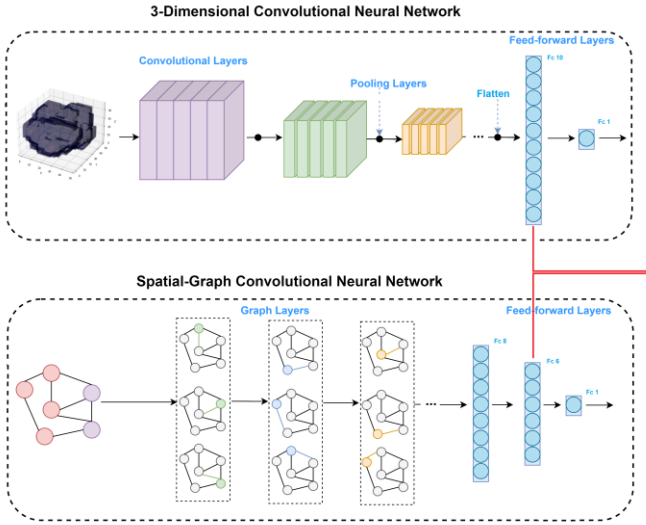


Fusion models for Atomic and molecular Structures developed by Lawrence Livermore National Laboratory [2]

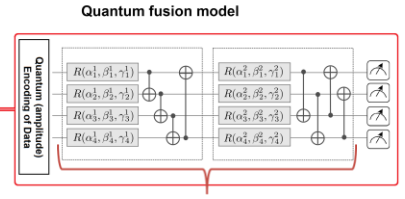


A protein-ligand binding complex

3. Our Hybrid Quantum-classical Fusion Model



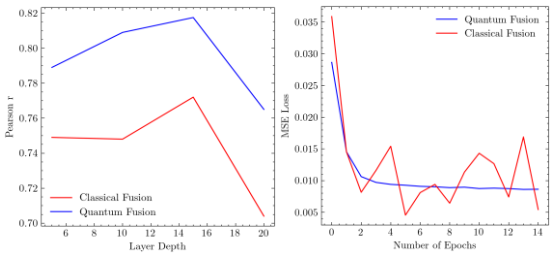
Outputs from second-to-last layer of the classical neural networks trained with the PDBbind dataset are encoded onto quantum states before being fed into a feed-forward quantum neural network (QNN).

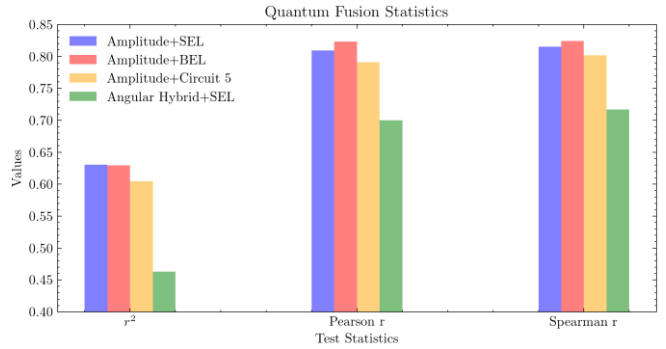


- Encoding schemes explored:
  - Hybrid angle, Amplitude
- Parametrized quantum circuits (PQC) explored in constructing the QNN:
  - Strongly Entangled Layers (SEL)
  - Basic Entangled Layers (BEL)
  - Circuit 5 from [3]
- ReLU activation layer after readout

4. Improved Results From Our Model

	r^2	MAE	Pearson r	Spearman r	RMSE
Classical	0.602	1.051	0.777	0.766	1.368
Quantum	0.630	1.040	0.809	0.815	1.295





References

[1] Guoli Xiong, Chao Shen, Zi-Yi Yang, Dejun Jiang, Shao Liu, Aiping Lu, Xiang Chen, Tingjun Hou, and Dongsheng Cao. Featurization strategies for protein–ligand interactions and their applications in scoring function development. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 12, 2021.

[2] Derek Jones, Hyojin Kim, Xiaohua Zhang, Adam Zemla, Garrett Stevenson, W. F. Drew Bennett, Daniel Kirshner, Sergio E. Wong, Felice C. Lightstone, and Jonathan E. Allen. Improved protein ligand binding affinity prediction with structure-based deep fusion inference. *Journal of Chemical Information and Modeling*, 61(4):1583–1592, 2021.

[3] Sukin Sim, Peter D. Johnson, and Alán Aspuru-Guzik. Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms. *Advanced Quantum Technologies*, 2, 2019.