Neural Network Model for Energy Prediction of Water Molecule

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Introduction-

Quantum neural networks involve combining classical artificial neural network models (which are widely used in machine learning for the important task of pattern recognition) with the advantages of quantum information in order to develop more efficient algorithms (ref. Wiki). In this report, I have discussed the advantage of using a neural network for predicting the energy of a specific configuration of the water molecule. I have used Keras (as referred in the tutorials) to build the model. To improve the accuracy of the model, I have increased the dataset from 1750 configurations to 3500 configurations. I have merged unrotated and rotated molecule configurations and created one big dataset to improve the deep learning of the model. While running the simulations for both datasets, I have observed few changes in the learning pattern of the model.

Observations-

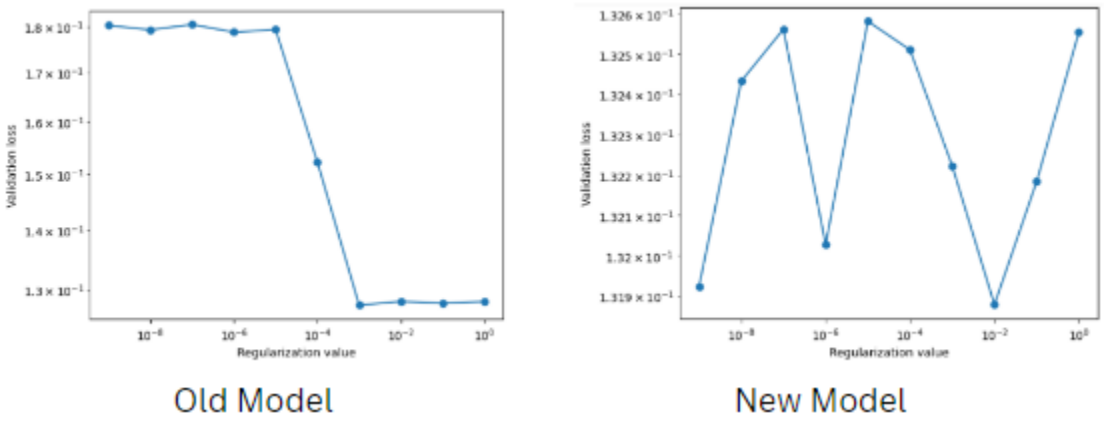
After merging the datasets, I have made certain observations about the predictions and the learning rate of the model. The first observation was made during training the dataset. The model mentioned in the tutorial had 1750 configurations, but as I have merged two datasets, the model is now trained using 3500 configurations. As the training data size of the model has increased, the model can make better predictions now. To train the model, I have used ~70% of the data size as training data, ~15% as validation data and ~15% as test data. The following are the observations made on the models learning and error rate-
(Note- Here when I say old model, I am referring to the model from the tutorial with 1750 configurations and the new model is the one with increased data size of 3500 configurations)

1. ***RMSE***- The models RMSE before increasing the dataset was 0.005149 and after increasing the dataset, the RMSE was 0.003448, the change is not major but given the fact that the model can be used for big data predictions, the error rate drop can be helpful in making better predictions

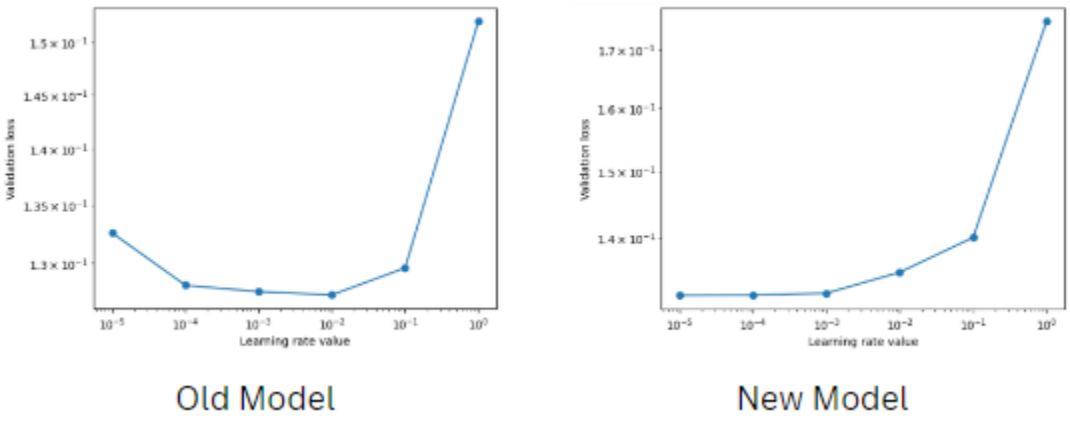
2. ***Regularization***- The regularization value as observed in the old model was 0.19 and as the model was trained, it went down to 0.14. The regularization value for the new model on the other hand is fluctuating slightly but is almost stable around ~0.132. This shows that regularization of the model got better after increasing the data size.

3. ***Learning rate***- The learning rate of the old model starts from around ~0.13 and goes up to ~0.15 whereas for the new model, the learning rate goes up to 0.17. There is a slight increase in the rate which signifies that the learning rate of the new model with larger dataset is better than the old model.

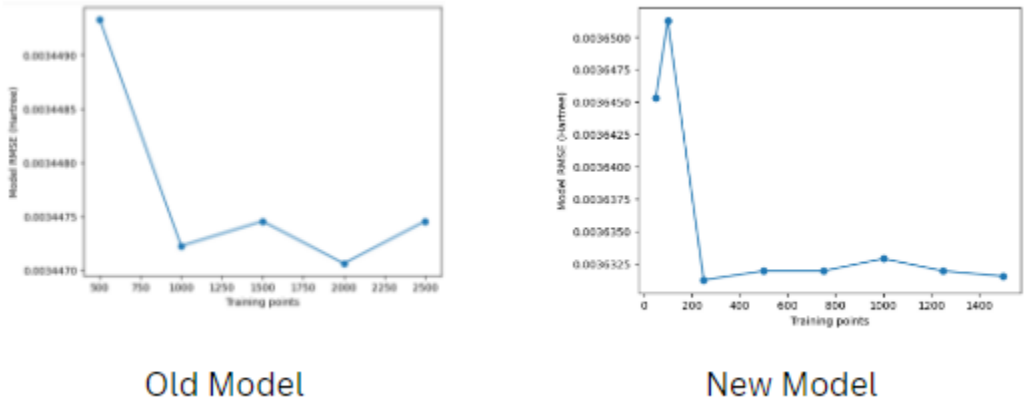
4. ***Learning curve***- The RMSE of the learning curve for the old model is around ~0.0036 while that of the new model is around ~0.0034. There is not much of a major difference in the RMSE value, but maybe with more data or while predicting for big data, the model might perform better when trained with a larger dataset.



(Fig) Regularization



(Fig) Learning rate



(Fig) Learning curve

Conclusion-

In summary, increasing the dataset or using a better training set can improve the accuracy of the model. After increasing the dataset, a ~65% error rate drop in the RMSE of the new model was observed which shows that there are significant advantages of improving the model's prediction by improving the dataset. By fine tuning the training dataset and the hyper parameters, the model's learning rate can be improved as well.

References-

[1] QML Slides by Prof. Alessandro Lunghi
[2] QML Tutorial by Dr. Ivan Rungger
[3] https://en.wikipedia.org/wiki/Quantum_neural_network