Results

Dereck Piché Guillermo Martinez Jonas Gabirot

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1 Results

1.1 Baseline: XGB

We trained and tested an Extreme Gradient Boosting (XGB) regressor using DNA sequences as features and their respective free-energy levels as labels. 900 000 samples were used for training and 100 000 samples for testing. The model's train and test performance were assessed by calculating the Mean Square Error (MSE) between the predicted and actual free energy levels given specific DNA sequences. 0.993166 and 1.016363 MSE were achieved on train and test evaluation respectively. These results will be used as baselines to evaluate further models' predictive performance.

1.2 Baseline: MLP

We built a standard MLP model as a deep learning baseline for our regression task. It consists of 21 fully connected layers. We trained the model on $900,000$ DNA sequences of length 30 and tested it's MSE loss on the remaining $100,000$ training examples. The DNA sequences were preprocessed into one hot encoded vectors of length 120. The accuracy troughout the epochs can be seen in figure 1.2

1.3 LSTM

We built a model using the regressive LSTM architecture for our regression task. Our regression LSTM is made up of a 2 LSTM layers and one fully connected layer. We trained the model on $900,000$ DNA sequences of length 30 and tested it's MSE loss on the remaining $100,000$ training examples. The DNA sequences were preprocessed into one hot encoded vectors of length 120. The accuracy troughout the epochs can be seen in figure 1.3

1.4 Regression Transformer

We built a model using the main components of the Transfomer architecture proposed in [1] for our regression task. Our regression transformer is made up

Figure 1: MLP loss

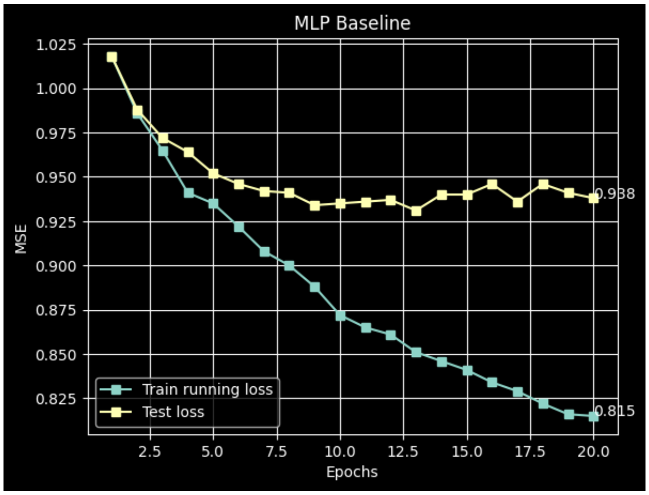


Figure 2: LSTM loss

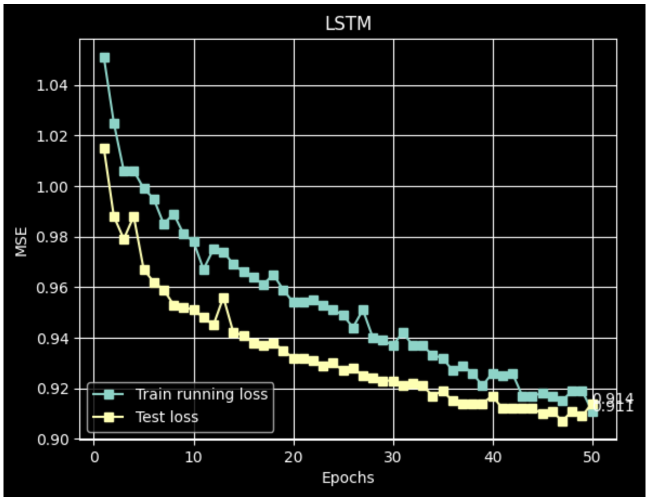
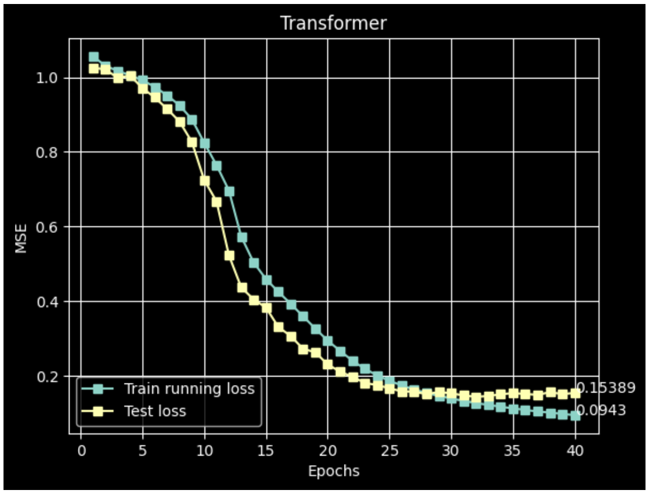


Figure 3: Transformer loss



of a sequence of encoder layers. Each of the encoder layers contains 8 attention heads with a ReLU activated linear layer. We trained the transformer on 900, 000 DNA sequences of length 30 and tested it's MSE loss on the remaining 100, 000 training examples. The transformer used the same positionnal encoding as the one proposed in [1]. The DNA sequences came in string form. Each of the 4 tokens were transformed into an integer and fed into a learned embedding layer that transformed them into vectors of 16 dimensions. The number of dimensions of the embeddings is a bit arbitrary, but since it works really well we left it there. The accuracy troughout the epochs can be seen in figure 1.4.

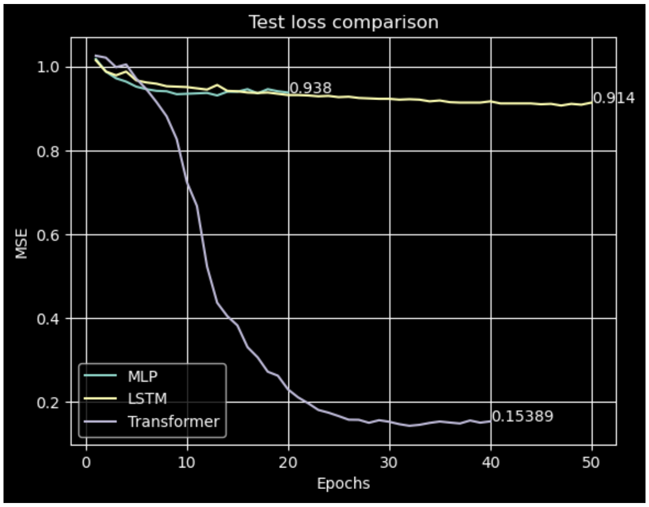
1.5 Comparison and analysis

We can see the comparison of the test loss in 1.5, where the regression transformer performs significantly better than the other models in their current state. In the final report, we shall augment the size of the other architectures in order to make them more competitive with the transformer, which has almost 2 million parameters. Furthermore, different statistical tools shall be applied to deepen our analysis, which is admittedly barebones at the moment.

2 Conclusion

We shall provide a conclusion in the final report, since our empirical data is lacking in volume to make definitive statements.

Figure 4: Loss comparison



References

[1] Ashish Vaswani et al. Attention is all you need. *CoRR*, abs/1706.03762, 2017.