A Neural Network approach to accelerate chemical kinetics codes

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Aim

In this era of exoplanet characterisation with JWST, the need for a fast implementation of classical forward models to understand the chemical and physical processes in exoplanet atmospheres is more important than ever. Notably, the time-dependent ordinary differential equations to be solved by chemical kinetic codes are very time-consuming to compute. In this study, we focus on the implementation of neural networks to replace mathematical frameworks in the one-dimensional chemical kinetics code VULCAN [1,2].

Methodology

Using the gravity gradient, temperature-pressure profiles, initial mixing ratios and stellar flux of a sample of hot-Jupiter's atmospheres as free parameters, the neural network is built to predict the mixing ratio outputs in steady state. The architecture of the network is composed of individual autoencoders for each input variable to reduce the input dimensionality, which is then used in an LSTM-like neural network to train this sequential data on.

Results

Results show that the autoencoders for the mixing ratios, stellar spectra, and pressure gradients are exceedingly successful in encoding and decoding the data. Additionally, for 90% of the cases, the fully trained model is able to predict the evolved mixing ratios of the species in the hot-Jupiter atmosphere simulations (figure 2). The fully trained model is 1000 times faster than the simulations done with the forward, chemical kinetics model while making accurate predictions.

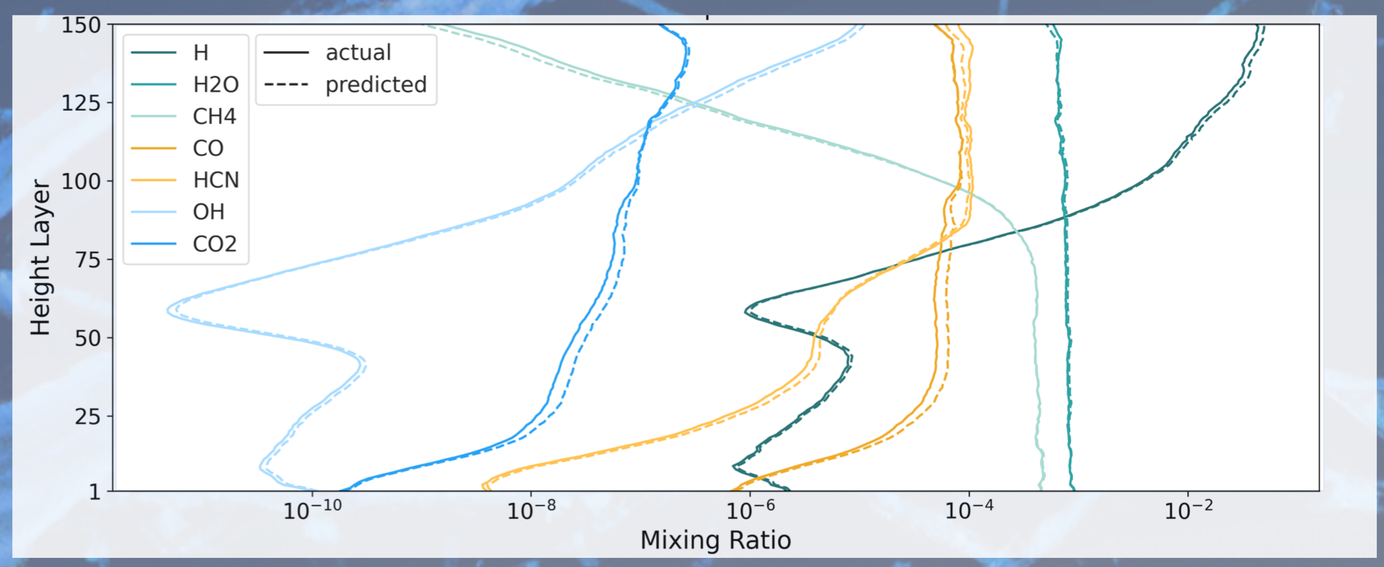

Figure 1. The mixing ratio per height layer for a selected set of species from an example of the dataset. The Solid lines show the actual mixing ratios as calculated by VULCAN, and the dashed lines show the neural network model predictions.

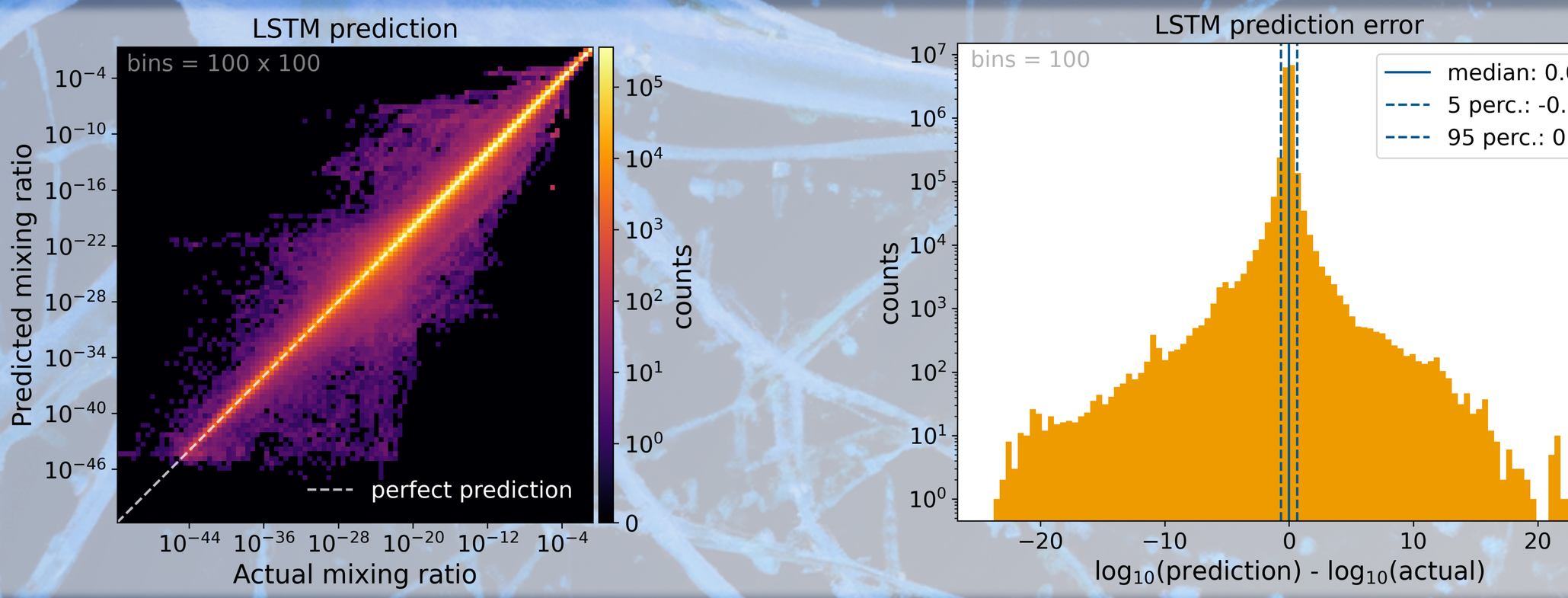

Figure 2. The LSTM predicted mixing ratios plotted against the actual mixing ratios (left) and the LSTM mixing ratio prediction error in log space (right). The dashed diagonal line in the left plot shows the performance of a perfectly predicting model and the colour of each bin represents the number of predictions. The solid line in the right plot shows the median value, and the dashed lines show the 5th and 95th percentiles.

Conclusion

In this work we replace the mathematical framework of solving ODEs in the chemical kinetics code VULCAN with a neural network approach. We found an accuracy of 90% where the fully trained model is able to predict the evolving mixing ratios. Using this model can reduce the computation times by 1000 times on average.

References

[1] S-.M. Tsai, J. R. Lyons, L. Grosheintz, et al. ApJs 2017
[2] S-.M. Tsai, M. Malik, D. Kitzmann, et al. ApJs 2021