Use of Neural Networks in estimating abundance of chemical species in Exoplanet atmospheres

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Abstract

To estimate the chemical abundances in exoplanet atmosphere, we need to employ disequilibrium chemistry techniques. This project investigates the possibility of replacing the chemical kinetics code used to calculate the mixing ratios with a neural network in order to reduce in atmospheric retrieval of an exoplanet when employing disequilibrium chemistry.

1 Introduction

To estimate the abundances of different chemical species in the exoplanet atmospheres, there are two methods, viz., first is by thermodynamic equilibrium and second by chemical kinetics. However due to certain processes like photochemistry disrupt the chemical equilibrium in exoplanet atmospheres and hence models with disequilibrium chemistry need to be employed that inherently involve chemical kinetics. This project aims replace the traditional method of estimating abundances using chemical kinetics by use of ML techniques.

2 Dataset Generation

The dataset required for the neural network will be generated using VULCAN. VULCAN is chemical kinetics code to calculate abundances of different species, and is governed by the following equations

$$\frac{\partial n_i}{\partial t} = \mathcal{P}_i - \mathcal{L}_i - \frac{\partial \phi_i}{\partial z} \tag{1}$$

where,

$$\phi_i = -K_{zz} n_{total} \frac{\partial X_i}{\partial z} \tag{2}$$

In the above equations, n_i, P_i and L_i denote the number density, production rate and loss rate of the ith species respectively and t denoters time. phi_i is the flux and X_i denotes the mixing ratio of the ith species (n_1 = X_i n_{total}). K_{zz} is the eddy diffusion coefficient.

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3 Implementation

3.1 Approach

In the method described by Hendrix et al. (2023), they assumed solar elemental abundances for the hot jupiters, that is, the planets for which the VULCAN code is valid. Along with that the eddy diffusion coefficient ($-K_{\text{zz}}$) was also kept constant when genereating the dataset.

This project aims to use the same idea for a single exoplanet. The Pressure-Temperature Profiles are generated by varying the elemental abundance. Then these PT profiles are used to generate the dataset using VULCAN. In the VULCAN configuration files four different eddy diffusion coefficients ($-K_{\text{zz}}$) were used to generate the data corresponding to each PT profile.

After generating the dataset, it is standardized as per the following equations,

$$p_s = \frac{\log_{10}(p) - \mu}{\sigma},$$

μ and σ are mean and standard deviation calculated by,

$$\mu = \frac{1}{n}\sum_{i=0}^{n} \log_{10}(p_i),$$

and

$$\sigma = \sqrt{\frac{1}{n}\sum_{i=0}^{n} (\log_{10}(p_i) - \mu)^2},$$

where,

$$p_{s,n} = \frac{p_s - \min(p_s)}{\max(p_s) - \min(p_s)},$$

3.2 Structure

In order to reduce the dimensionality of the input data points autoencoders have been employed. For each of the six properties mentioned above, an autoencoder has been used.

Grassi et al. (2022) have also shown that autoencoders can be sucessfully used to reduce the complexity of the chemcial networks.

The loss function to determine the performance of the autoencoders is defined by

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N} \left(\frac{p_i - a_i}{a_i}\right)^2 \tag{3}$$

where p_i and a_i respectively are the predicted and actual vectors.

The purpose of the autoencoders is to reduce the dimensionality and the complexity, eventually reducing training time. The core network is made to learn the mapping from the input properties to the evolved output from VULCAN. AS VULCAN evolves with time by solving ODEs, an LSTM-like neural network is chosen as the core network to account for time evolution. (Hendrix et al., 2023). The LSTM neural network is special case of RNN (Recurrent Neural Network) that has a complex architecture comprising of four gates, viz. forget gate (discards useless information), learn gate (learns new information), remember gate (retains necessary information) and output gate. LSTM can also overcome vanishing gradient problem for small sequential data with the help of these gates.

To gain more accuracy and impart the sense of time evolution the output from the core network is again feeded to the core network. This would help in improving accuracy theough the different time steps to finally generate the mixing ratios in the exoplanet's atmosphere.

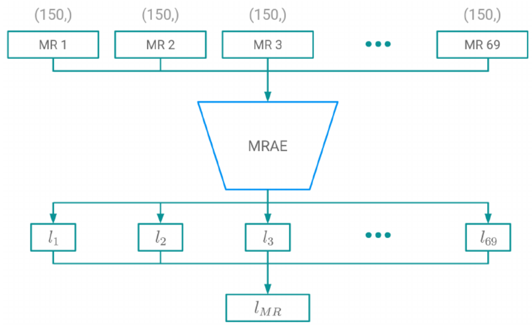

Figure 1: Illustrative representation of autoencoder for the mixing ratios for 69 species for 150 layers in the atmosphere.

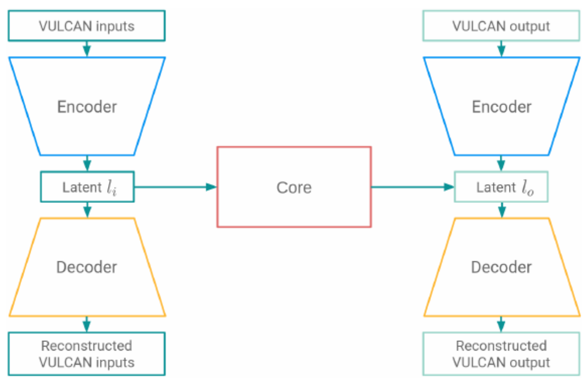

Figure 2: Illustrative representation of the full neural network

3.3 Future Plans

To succesfully use idea discussed in the report to develop a neural network that would replace the VULCAN code in the atmospheric retrival of an exoplanet.

References

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