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

Sarthak Patel

School of Physical Sciences
National Institute of Science Education and Research,
Bhubaneswar
sarthak.patel@niser.ac.in

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 by much faster ML technique using neural networks.

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

$$\frac{\partial n_i}{\partial t} = P_i - L_i - \frac{\partial \phi_i}{\partial z} \quad (1)$$

where,

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

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

Please pay special attention to the instructions in Section 3.1 regarding figures, tables, acknowledgments, and references.

As described in Hendrix et al., the dataset is generated by varying the following parameters:

1. Planet's Mass within the range [0.5, 20] M_J
2. Orbit Radius within the range [0.01, 0.5] AU

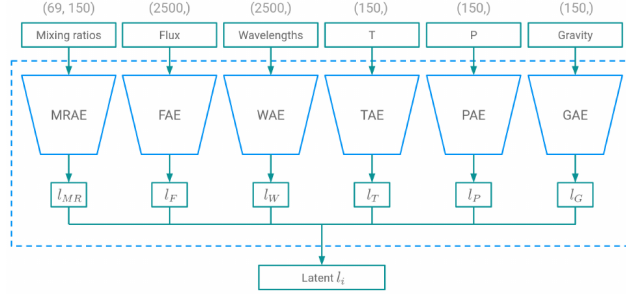


Figure 1: Illustrative representation of input properties with their respective autoencoders

3. Stellar Radius within the range $[1, 1.5] R_{\odot}$
4. Planet Radius
5. Temperature-Pressure Profile
6. Stellar Flux

3 Implementation

3.1 Input Parameters

For the input to the neural network, six properties were chosen at the initial condition of VULCAN.

1. Initial mixing ratios (the mixing ratios for 69 species are defined for the 150 height layers of the exoplanet atmosphere)
2. Temperature Profile (150,)
3. Pressure Profile (150,)
4. Gravitational Profile (150,)
5. Stellar Flux (2500,)
6. Stellar Wavelength Component (the corresponding wavelength for the stellar flux from the stellar spectrum) (2500,)

3.2 Structure

From the above list of properties we have, for each configuration, $(69 \times 150 + 150 + 150 + 1500 + 2500 + 2500)$ data points. 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 successfully used to reduce the complexity of the chemical networks.

3.2.1 Core Network

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)

3.3 Future Plans

As discussed in the above sections, the neural network is designed to work for a generalized set of planets as validated by VULCAN, however, in order to generalize the estimation of chemical abundance, some of the properties are taken on the basis of certain of assumptions, viz., for the hot-Jupiters it is assumed that they have solar elemental abundance, the eddy diffusion constant is kept constant.

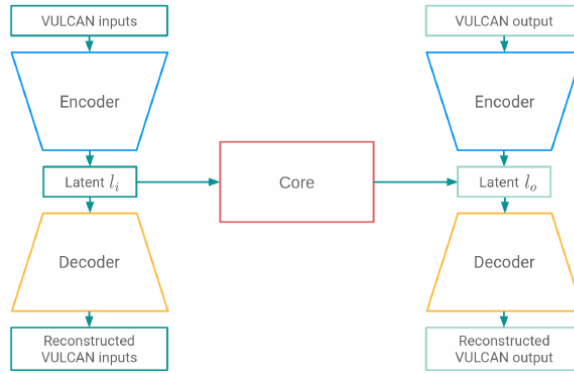


Figure 2: Illustrative representation of the full neural network

To use this idea in the atmospheric retrieval of an exoplanet, we vary the elemental abundances that would in turn generate different Temperature-Pressure Profiles and also varying the eddy diffusion constant, hence modifying the input properties to apply the neural network method to an exoplanet. The plan is to explore this idea and possibly implement a neural network.

References

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- [3] Tsai, S. M., Lyons, J. R., Grosheintz, L., Rimmer, P. B., Kitzmann, D., & Heng, K. (2017). VULCAN: an open-source, validated chemical kinetics python code for exoplanetary atmospheres. *The Astrophysical Journal Supplement Series*, 228(2), 20.