Using NN in estimate abundance of different species in an exoplanet atmosphere

Sarthak Patel
School of Physical Sciences, National Institute of Science Education and Research, Bhubaneswar, India
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Instructor - Dr.Shubhankar Mishra

Introduction

There are two approaches that are commonly used to estimate the abundances of species in an exoplanet's atmosphere. First method is by thermochemical equilibrium. The second method is by use of chemical kinetics to generate chemical disequilibrium models that take into account processes like photochemistry, etc. The former method is fast as it does not require an extensive list of reactions between different species, unlike the second method. Thus the employing disequilibrium chemistry makes it computationally expensive. This project investigates the neural network implemented by Hendrix et al., 2023 and explores the possibility of implementing the same for a single exoplanet.

Idea

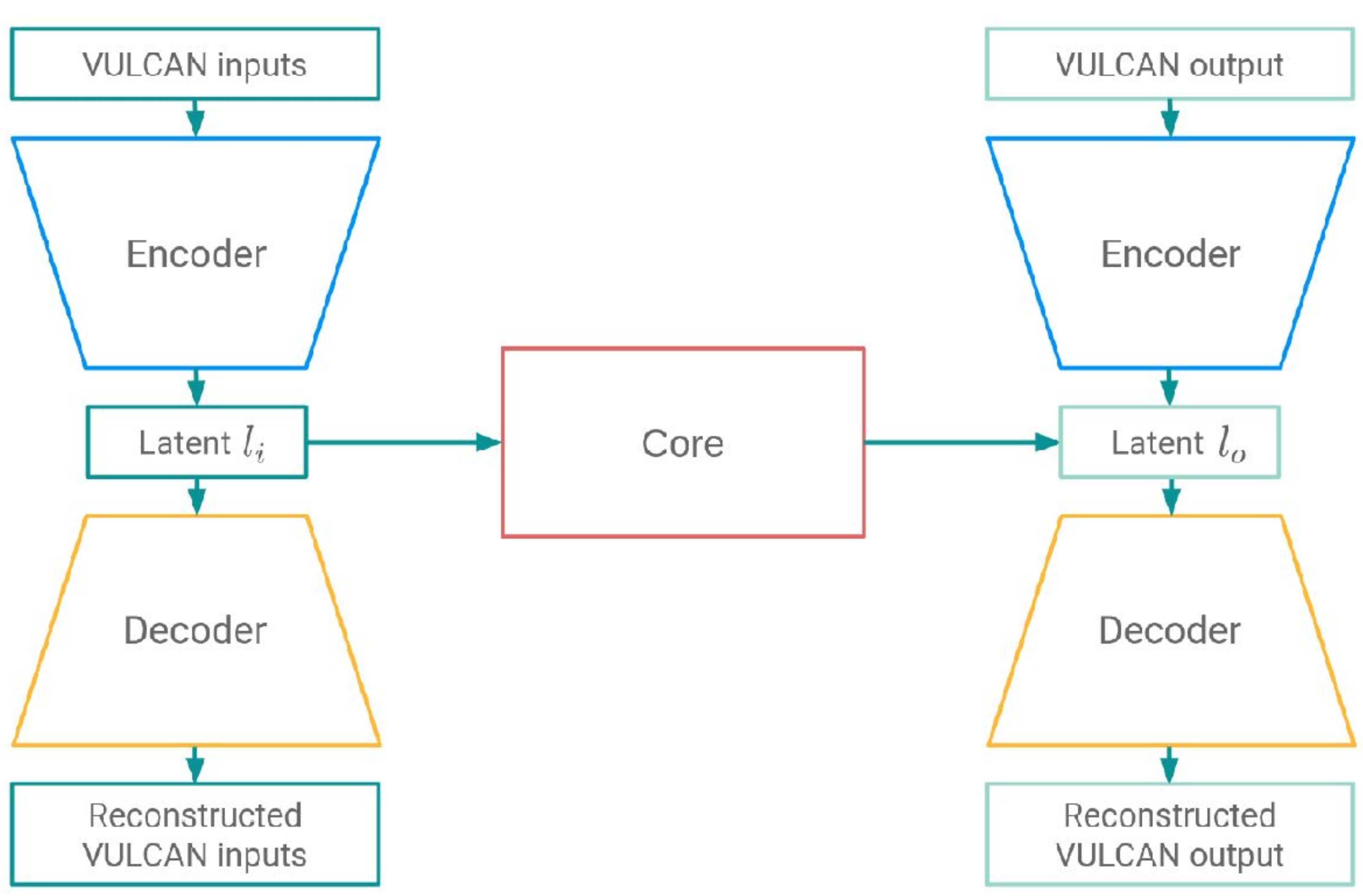
- Traditionally, the abundancees of different species can be estimated using chemical kinetics code that solves ODEs and takes into account the chemical reactions between different species using an existing code VULCAN (Tsai et al., 2017)
- The objective is to achieve sufficient accuracy as VULCAN code by using Machine Learning Techniques. This project discusses one such method implemented by using neural networks.

Autoencoders

- Autoencoders are employed to reduce the dimensionality of data. This also helps in reducing the training time and complexity.
- It consists of an encoder and a decoder. The input data is feeded to the encoder that encodes the the data to lower dimensionality representation, also called as the latent representation.
- The decoder takes the data in latent representation and then reconstructs the original data.

Core Network

- The Core network takes the latent representations a s the input and maps to the evolved output from VULCAN. After this the output is passed to the decoder to generate the final evolved mixing ratios.
- The abundances in terms of mixing ratios is calculated by solving ODEs . So, to impart this time sense and evolution , the core network is based on LSTM neural network.



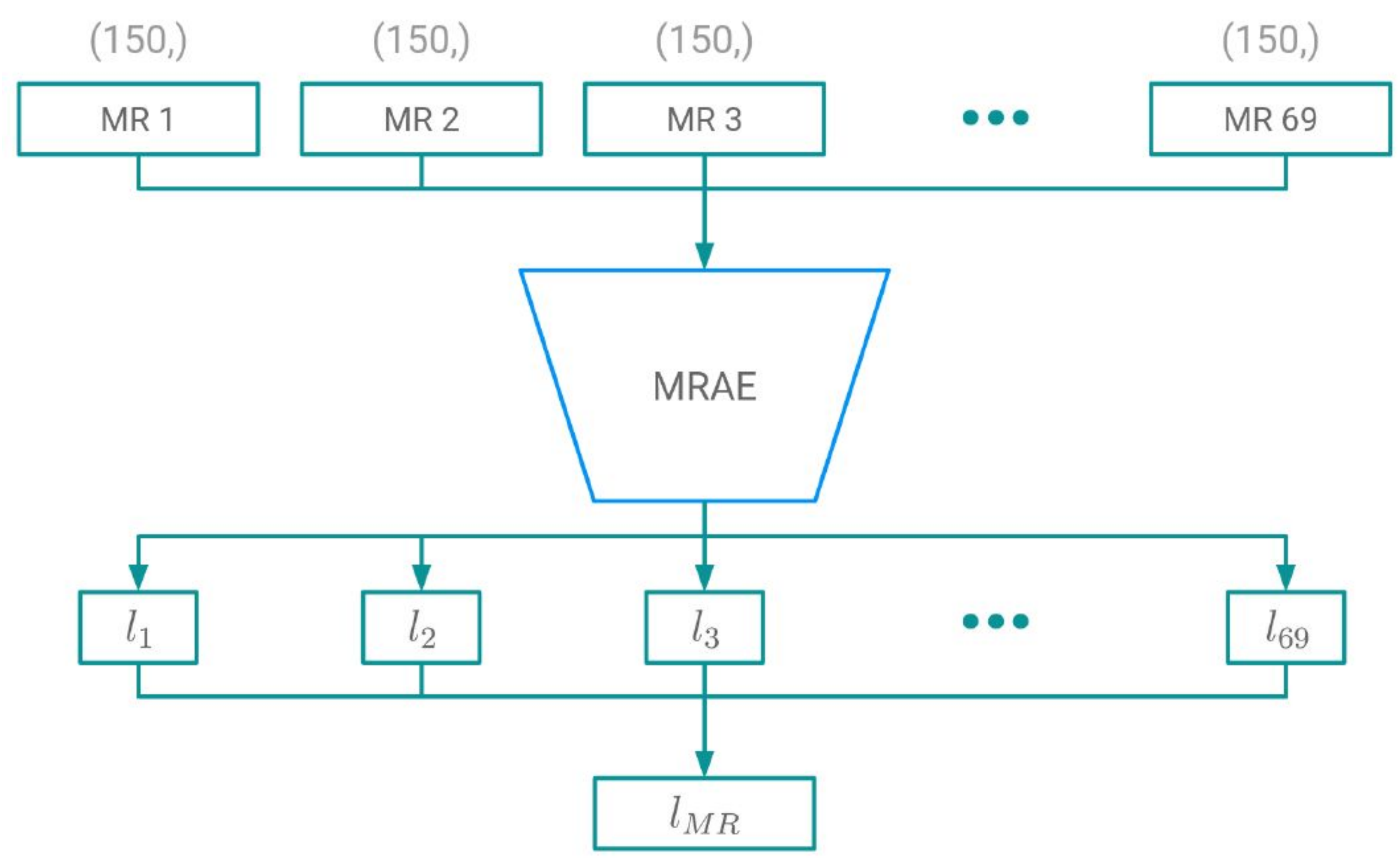
Schematic of Autoencoder for Mixing Ratios of different species

Input Properties

- The input properties comprise of initial mixing ratios, pressure profile, temperature profile. These properties have different scales, hence it is necessary to standardize them. ,

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

$$\sigma = \sqrt{\frac{1}{n}\sum_{i=0}^{n}(\log_{10}(p_i) - \mu)^2}, \qquad p_{s,n} = \frac{p_s - \min(p_s)}{\max(p_s) - \min(p_s)}$$



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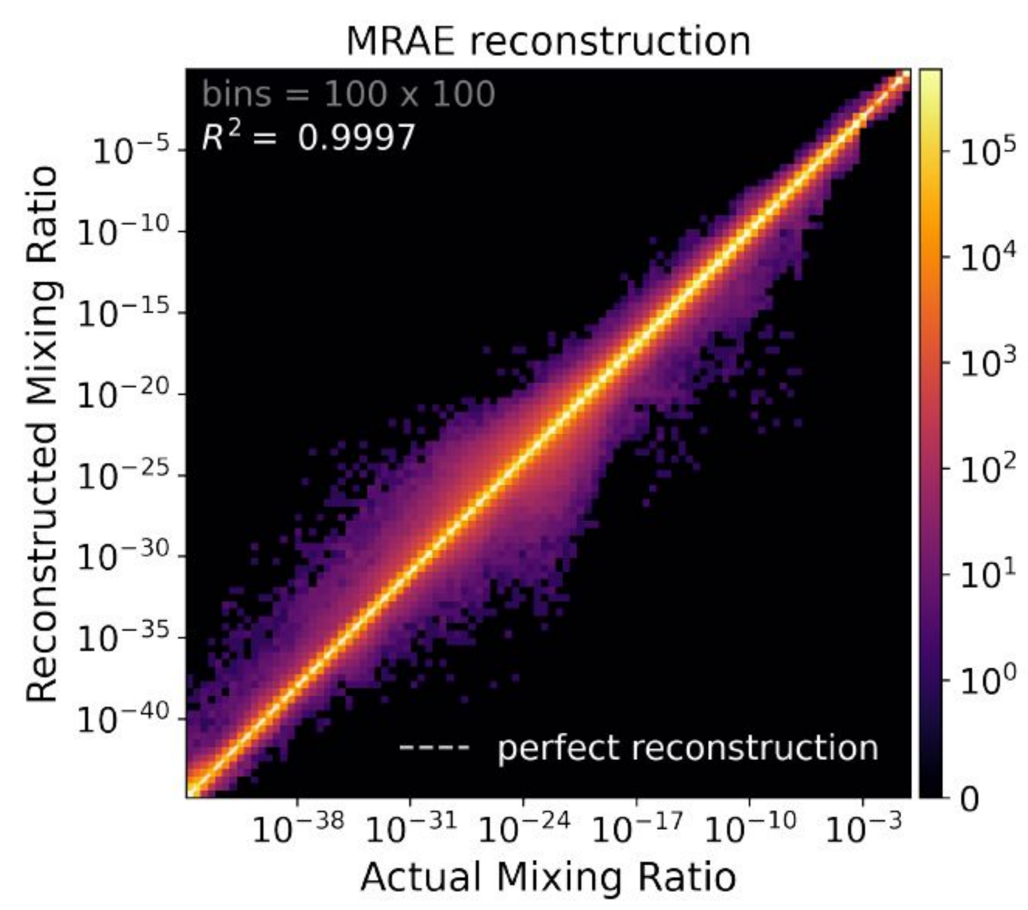

Performance of Autoencoder for Mixing Ratios of different species (Hendrix et al. (2023)

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