Testing our ML P-T Model in an Atmospheric Retrieval

We validated that our **ML P-T model (two parameters)** outperforms a classical **4th order polynomial P-T model (five parameters)** in a retrieval. For each P-T model we ran one retrieval on the simulated mid-infrared **emission spectrum of an Earth-like planet orbiting a Sun-like star** at a distance of 10 pc (spectral resolution $R = 200$, photon-noise signal-to-noise ratio $S/N = 10$ at 11.2 μm). In addition to the P-T profile parameters, we retrieved **for 10 additional parameters**, including the planet's radius, and the mass fractions of different atmospheric gases.

The results from this retrieval test are shown in **Fig. 3** (retrieved P-T profiles) and **Fig. 4** (residuals of fitted spectra). We find:

4. The spectrum residuals in Fig. 4 show that **both retrievals accurately reproduce the Earth-like spectrum**, despite the differences in the P-T models. Both residual are centred on truth, and are significantly smaller than the 1 σ noise level.

1. The P-T structure of the atmosphere is **retrieved better with our ML P-T model than with the polynomial baseline**. At high pressures ($\geq 10^{-3}$ bar), the ML P-T model accurately reproduces the true P-T profile. At low pressures (<10-3 bar), the ML P-T model tends to underestimate the true temperature. Since low pressure regions do not contribute strongly to the exoplanet's spectrum (see contribution function in Fig. 3), the low pressure regions are hard to constrain in retrievals.

2. Form the inlay plot in Fig. 3, we see that our ML P-T Model **yields better constraints for both surface pressure P₀ and the surface temperature T₀**. Especially the P₀ constraint is stronger and less biased than for the polynomial baseline.

3. The retrieval results for the additional **non-P-T parameters show no strong dependence on the choice of P-T model**.

5. The retrieval using **our ML P-T model was significantly faster than the polynomial baseline** due to the reduced number of P-T profile parameters. The total runtime was reduced by an approximate factor of 3.2.

We highlight two benefits of our ML P-T model. First, it **reduces the number of P-T parameters** in retrievals, which lowers the computational cost and allows to retrieve additional parameters of interest. Second, it allows us to **use more realistic physically consistent P-T profiles in retrievals**.

Learning-Based Pressure-Temperature Model

One key component of an atmospheric retrieval is the **pressuretemperature (P-T)** profile. It describes the thermal structure of the atmosphere. Simple functions (e.g., polynomials [1,2]) are commonly used to model the P-T profile. Such models require a large number of parameters (increases retrieval runtime) and **may produce unphysical P-T structures**.

¹ Institute for Particle Physics & Astrophysics, ETH Zurich \parallel ² National Center of Competence in Research PlanetS \parallel ³ Max Planck Institute for Intelligent Systems, Tübingen *Attending the Planet-ESLAB-2023 conference on-site

We devised a **Machine-Learning (ML)** approach for **a physically consistent P-T profile model**, which requires fewer parameters than classical P-T models (**Fig. 1**). We train our ML model on P-T profiles from the PyATMOS dataset [3], which consists of 124'314 physically consistent P-T profiles (generated with Atmos [4,5]) of **Earth-like planets orbiting solar-type stars**. During training, our ML method uses an encoder network E to map the P-T profiles in the training dataset onto a set of N **latent variables z**_i (here, we use N=2). We then use the z_i to train a decoder network D, which generates a **P-T structure corresponding to a set of zi** . During training, we condition D such that it minimizes the difference between the P-T profiles from the PyATMOS dataset and the ones that it generates from a set of z_i . When running retrievals, **we use D to generate P-T profiles for zi values** proposed by the Bayesian parameter estimation routine.

Background – Atmospheric Retrievals

An **atmospheric retrieval** finds the best fit of a model for the exoplanet's spectrum to the observed spectrum. Additionally, it retrieves Bayesian **estimates and uncertainties for the model parameters (Fig. 2)**. These model parameters describe the exoplanet's bulk and atmospheric properties, such as the exoplanet radius, the pressure-temperature structure, the surface conditions and the abundances of atmospheric gases. Our retrieval routine [1,2] relies on two subroutines:

- 1. A **radiative transfer code** (petitRADTRANS [6]) to calculate the spectrum corresponding to a 1D atmosphere structure described by a set of model parameter values.
- 2. A **Bayesian parameter estimation routine** (MultiNest [7] via pyMultiNest [8], which is based on Nested Sampling [9]), to find the set of parameters (with uncertainties) that best fits the observed spectrum.

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 H_2O O_3 CO_2

Improving Exoplanet Atmospheric Retrievals with a Learning-Based Pressure-Temperature Profile Model

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B.S. Konrad^{1,2}, T.D. Gebhard^{1,3}, D. Angerhausen^{1,2,*}, E. Alei^{1,2}, S.P. Quanz^{1,2,*}, and B. Schölkopf³

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Contact Me: konradb@student.ethz.ch

Personal Website: https://konradbjorn.github.io

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Figure 3: Left: P-T profile retrieved from the MIR thermal emission spectrum of an Earth-like planet for different P-T models (purple areas – our ML P-T model; blue lines – polynomial P-T model [1,2]). The inlay in the top-right corner shows the retrieved surface conditions. Right: Contribution of different atmospheric layers to the Earth-like thermal emission spectrum.

Figure 4: Relative difference between the Earth-like spectrum and the spectra corresponding to the retrieved parameter values. ([true spectrum - simulated spectrum]/true spectrum). Top: retrieval using our ML P-T model; Bottom: retrieval using a polynomial P-T model [1,2].

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