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The Bayesian Atmospheric Radiative Transfer (BART) Code in the JWST Era

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Abstract

Bayesian Atmospheric Radiative Transfer (BART, [1], [2], [3]) is an open-source, reproducible-research code for atmospheric composition and structure retrieval. Its Bayesian sampler [4] proposes atmospheric models and compares them to data via a line-by-line radiative-transfer (RT) code. Auxiliary codes initialize to thermochemical equilibrium [5], produce plots and diagnostics, calculate contribution functions, etc. The BARTTest module checks validity against known-correct calculations or community consensus results, depending on the test. BART has modes for eclipse, transit, and isolated objects (such as imaged exoplanets, solar-system atmospheres, or brown dwarfs). BART is currently a 1D code. Clouds are being implemented. In preparation for new observatories like the James Webb Space Telescope, Ariel, and large ground-based telescopes, we are adding a 3D mapping capability. Due to efficiency concerns, we are implementing a machine-learning-based RT routine. Because of the complexity of retrieval studies and difficulty in reproducing them, several unnecessary controversies have blown up around retrieval questions. We propose reproducible research (RR) guidelines for retrieval papers. BART's license requires that users follow RR practices in reviewed publications.

1. Introduction

"Retrieving" (inferring) atmospheric properties from observations requires fitting a complex model to data. For exoplanets, the signal is immersed in stellar noise and may be weaker than instrumental systematic errors. To explore the model phase space well enough to assessm parameter uncertainties and correlations, investigators turn to Bayesian methods. Several codes now implement this approach (see, e.g., [6], and references therein). As larger telescopes and purpose-built instruments improve data, we wish to reduce the model's simplifying assumptions. One such assumption, made due to practical rather than physical considerations, is that a single atmospheric composition and thermal profile characterize an entire planetary dayside or limb region, despite logic and models demonstrating otherwise.

BART imposes few physical constraints, allowing the data to speak. However, if the real planet has regions with different compositions due to progressive dayside photochemistry under circulating winds or simply to varying temperatures, a 1D model planet could indicate an implausible composition.

2. BARTTest

Given the calculation's complexity, good practice requires rigorous testing, including isolating components of the calculation and comparing to known or consensus-based answers. To ensure the quality of BART, it contains a small, simple code, MiniRT, written in Python, that implements its core physics. This is the basis of the BARTTest module, whose tests include single, separate, and blended lines in single and multiple layers, for detailed comparison to the known Voigt profiles; an isothermal atmosphere for comparison to the Planck function; and complex atmospheres, to be compared to the results of other codes. The initial comparison is to co-author IDD's RT code.

3. 3D

Using Spitzer images, [7] and [8] made location-dependent thermal or compositional maps. The brightness source was ambiguous: was it hotter in the bright region, or was there a higher abundance of the emitting gas? With JWST observing limb-crossing by the most favorable eclipsing hot Jupiters, spectroscopy can break this degeneracy. Prior to JWST launch, we plan to extend BART to run retrievals over a 3D grid of thermal profiles and a 2D or 3D grid of compositions. To reduce the number of free parameters, a functional form will force parameters to change slowly with location.

4. Fast RT with Machine Learning

Such a calculation would multiply runtimes by the number of RT columns. For efficiency, we are now training a deep neural network as a surrogate RT model. Once trained, this model will run many times faster than standard RT, without sacrificing a fully Bayesian approach.

5. Reproducible Research

The retrieval calculation has too many details to mention all of them in a paper of reasonable length, making reproducibility difficult. This is common in all disciplines involving computer programs, and has spawned the Reproducible Research (RR) movement. RR advocates that each paper be co-published with a compendium of codes, data, settings, and outputs supporting the claims in the paper. Others may then inspect the calculation and even re-run the code to verify the result. We propose [1] RR best practices for retrieval papers, and BART's license requires that users follow these in refereed reports. We encourage investigators to consider adopting RR practices for all their papers.

6. Summary and Conclusions

BART's code and documentation is available on GitHub (https://github.com/exosports/BART). The package is well documented and there is a support mailing list. The included BARTTest code can be applied to any RT or retrieval code, and we seek additional tests and comparison-test results via Git pull requests. Currently, BART implements a 1D model. A cloud capability is in development, as is acceleration through machine learning-based RT. Our plans include the capability to map eclipsing exoplanet atmospheres in 3D.

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