The Need for Speed (and Accuracy): Surrogate Models in Exoplanet Atmospheric Characterization

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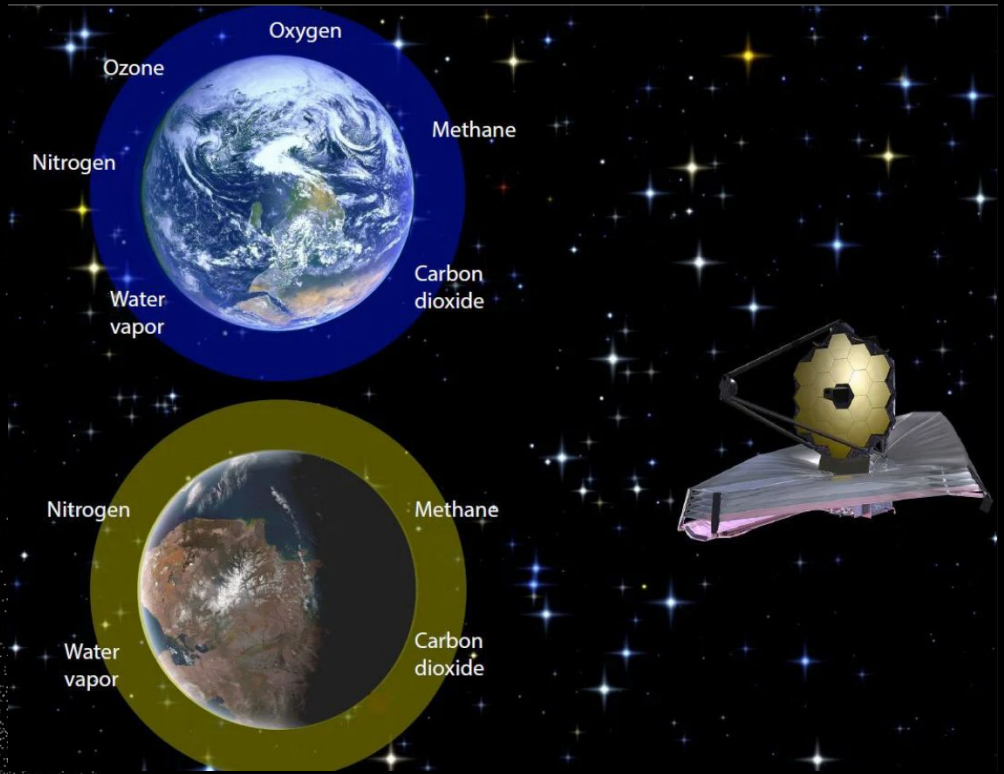
What are exoplanets and why do we study their atmospheres?

- Exoplanets: Planets that orbit stars outside our solar system
- Understanding the atmospheric conditions is crucial in determining the planet's habitability [1]
  - Find and quantify the constituents of the atmosphere and planet's surface
- But there is only so much we can do with observations and the vast amount of data they produce

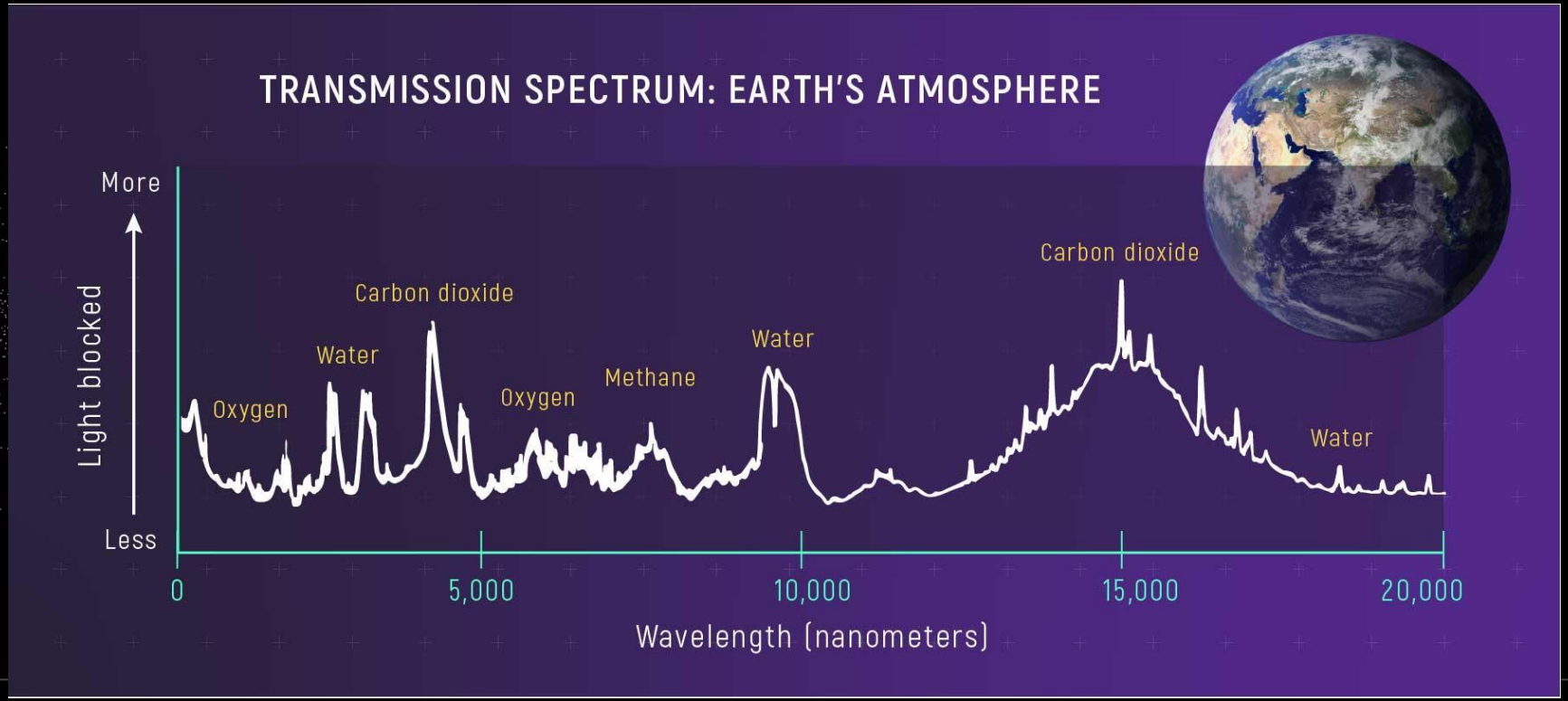


Credit: NASA/Wikimedia Commons/Joshua Krissansen-Totton

[1] Madhusudhan & Seager 2009, ApJ 707, 24.

How do we study their atmospheres?

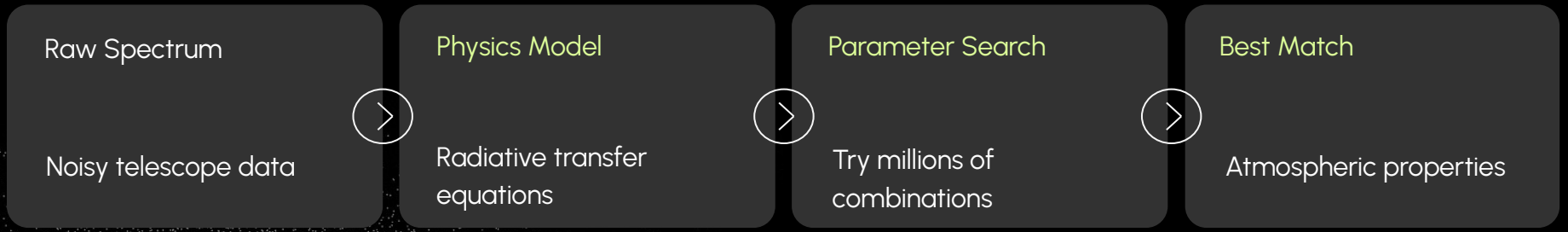
We analyse the light that passes through or comes from their atmospheres.



Credit: NASA, ESA, and L. Hustak (STScI).

How do we gain insights from it and the challenge?

Getting from raw spectrum to atmospheric composition is incredibly complex.



- **Complex Physics:** Must solve radiative transfer through entire atmosphere
- **Many Parameters:** Temperature, pressure, molecular abundances at many layers
- **Statistical Sampling:** Need millions of model runs to find best fit
- **High Precision Required:** Tiny signals need careful analysis

Result: Very accurate results based on solid physics! [2]

Hours to days per planet!
Computationally expensive
Limited for large surveys

[2] Himes et al. 2022, PSJ 3, 91.

Enter Machine Learning Surrogate Models

Simplified approximations of more complex, higher-order models

The main idea:

- Train neural network on thousands of synthetic atmospheric spectra
- Learn patterns between atmospheric properties and light signatures
- Make rapid predictions on new observations
- From hours to minutes! [3]

But can we maintain accuracy while gaining speed?

[3] Benneke & Seager 2012, ApJ 753, 100.

Our approach

- Step 1: Generate Training Data
  - Generated synthetic atmospheric spectra using Markov Chain Monte Carlo (MCMC) coupled with radiative transfer code, petitRADTRANS [3]

Credit: petitRADTRANS

- Step 2: Train and Optimize Neural Network
  - Trained separate transmission- and emission only neural surrogate models using MARGE library on the synthetic spectra dataset [2] (Took us ~9.5 minutes)
  - **Fine-tuned the model to handle noisy data and avoid generalization**
- Step 3: Test on Real Exoplanets
  - Compared synthetic transmission and emission spectra predictions with observational data of exoplanets HD 189733 b and GJ 1214 b [4, 5]

[2] Himes et al. 2022, PSJ 3, 91. [3] Benneke & Seager 2012, ApJ 753, 100. [4] Kempton et al. 2023, Nature 620, 67. [5] Zhang et al. 2025, AJ 169, 38

What did we find? (1 of 3)

Transit depth → planet blocked starlight

Model-data mismatch

Model does not fit well

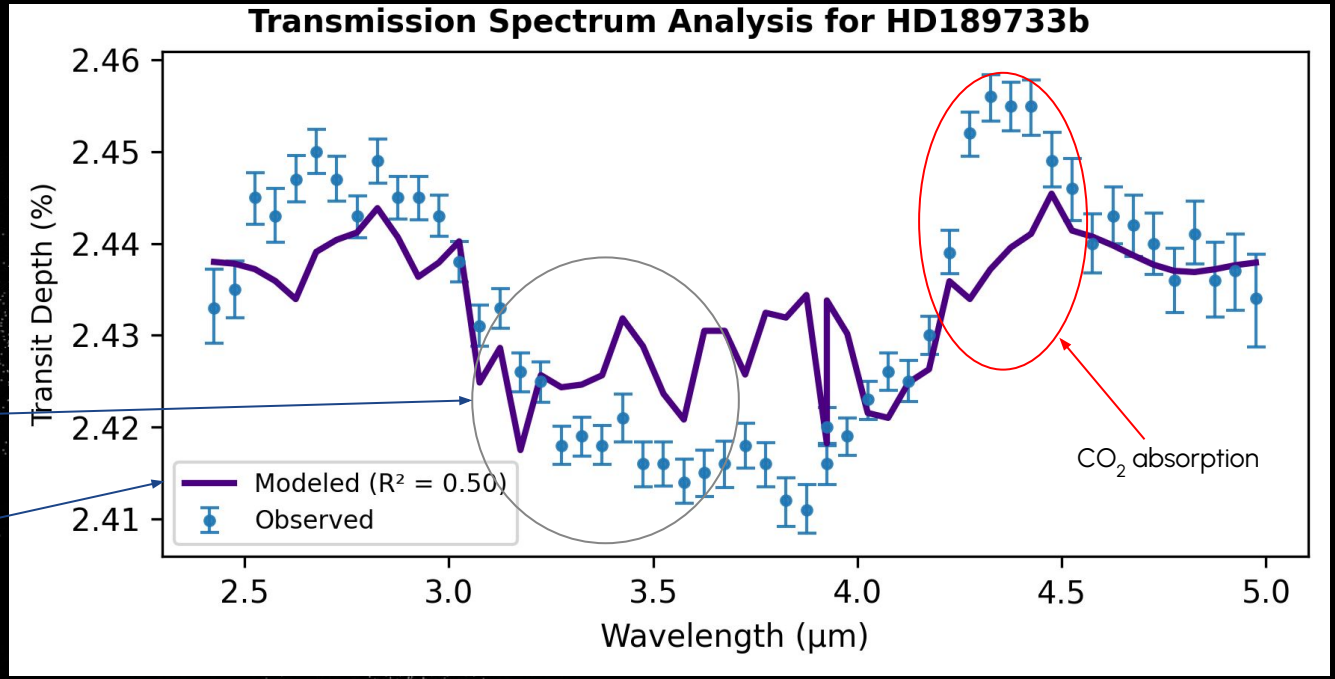


Fig. 1: Transmission spectra for HD 189733 b (2.5-5.0 μm). Model (R^2=0.50) vs. observed atmospheric absorption data.

What did we find? (2 of 3)

Higher R^2, stronger model fit

Secondary eclipse → planet's thermal emission

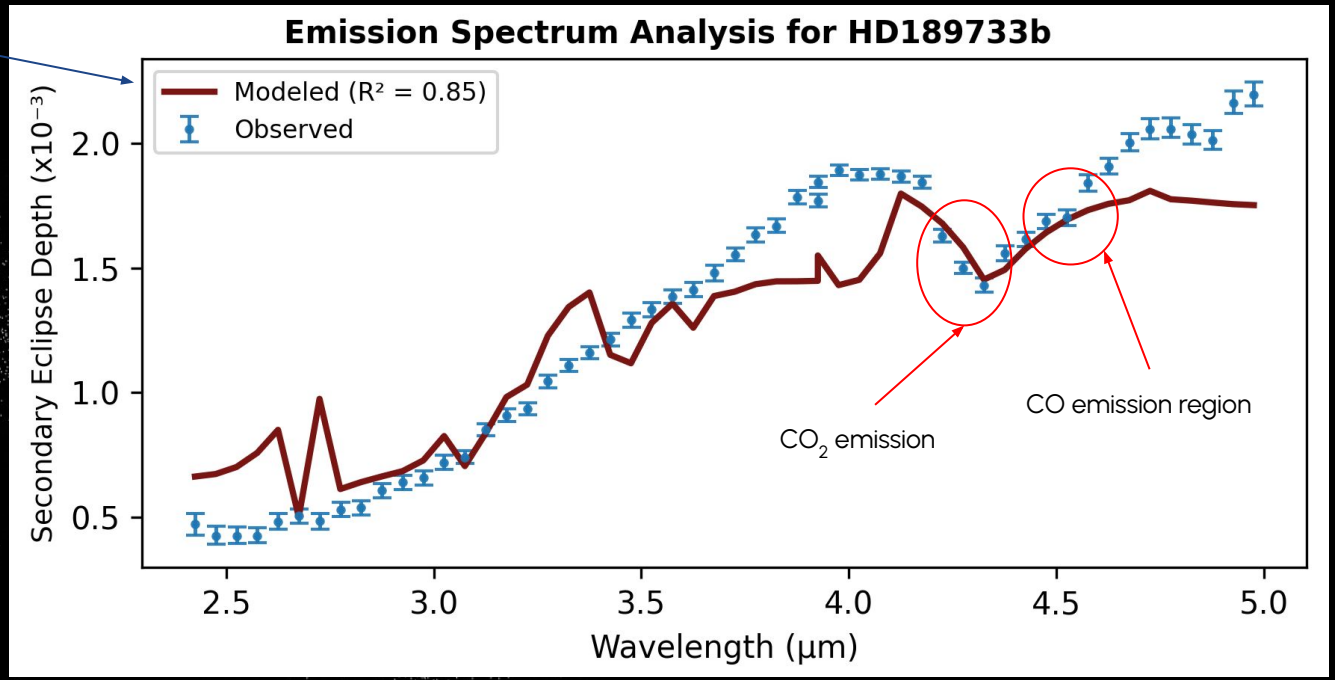


Fig. 2: Emission spectra for HD 189733 b (2.5-5.0 μm). Model (R^2=0.50) vs. observed thermal emission data.

What did we find? (3 of 3)

Higher R^2, stronger model fit

Secondary eclipse → planet's thermal emission

Four modeling approaches

Model spread

All models agree

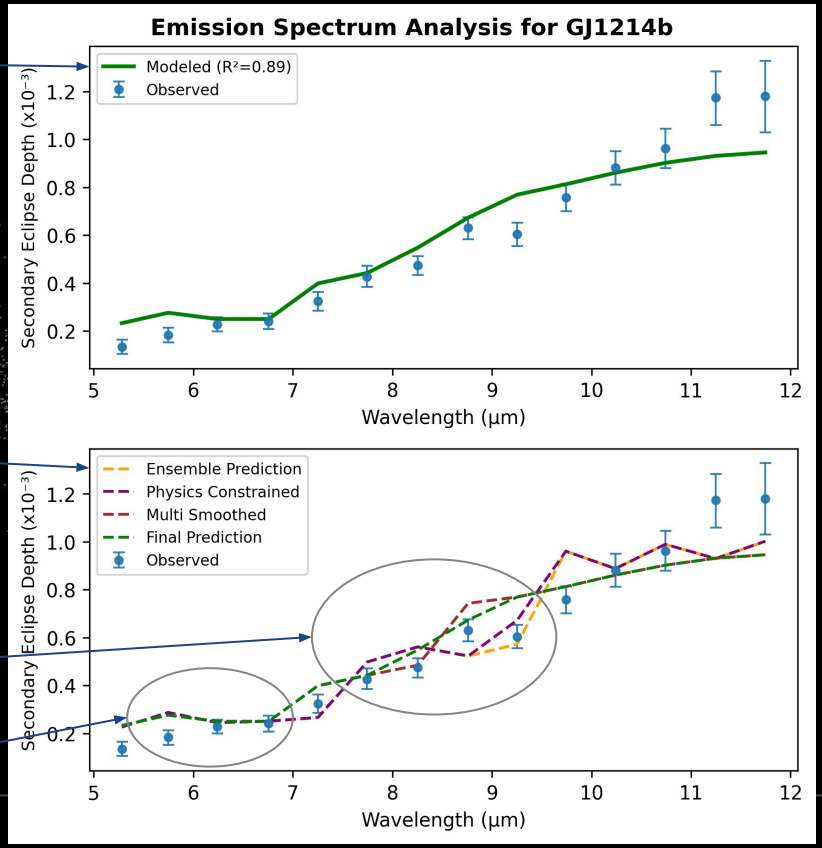


Fig. 3: Emission spectrum for GJ 1214 b (5-12μm). Top: Best-fit model vs. observations. Bottom: Comparison of four modeling approaches (ensemble, physics-constrained, multi-smoothed, final prediction) with observational data

What does this imply?

- Surrogate models accurately recover emission spectra (R^2 = 0.85-0.89) but show moderate performance for transmission spectra (R^2 = 0.50).
- Physics-informed constraints (radiative transfer principles, molecular opacities) and ensemble methods improve model reliability.
- Models successfully identify atmospheric molecules (CO_2, CO) in both emission and transmission observations.
- Results demonstrate surrogate models as fast, reliable tools for emission retrieval (~9.5 min vs. hours), with transmission modeling requiring further development.

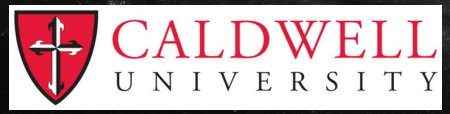
[2] Himes et al. 2022, PSJ 3, 91. [3] Benneke & Seager 2012, ApJ 753, 100. [4] Kempton et al. 2023, Nature 620, 67. [5] Zhang et al. 2025, AJ 169, 38

What's next?

- Incorporate physics-based constraints to improve transmission modeling and generalize across diverse exoplanet types.
- Work on model interpretability
- Develop user-friendly tools for astronomers

Thank you for your attention!

Any questions?



Bonus Slides!

Model Architecture

Neural Network Design:

- 2 Convolutional layers (pattern recognition)
- 4 Dense layers (decision making)
- ReLU activation functions
- Spectral-weighted loss function

Training Details:

- 14,000 total spectra (10k train, 2k validation, 2k test)
- 250 training epochs
- Channel-wise normalization
- Targeted regularization to prevent overfitting

Why is transmission spectroscopy harder?

Emission (Easier)

- Strong signal from hot planets
- Direct thermal glow
- Less atmospheric complexity
- More predictable patterns

Transmission (Harder)

- Weak signal - tiny atmospheric layer
- Complex scattering effects
- Cloud/haze contamination
- Limb temperature variations

Atmospheric characterization is the key to finding habitable worlds.

Biosignature Gases We Look For:

- Water (H_2O): Essential for life as we know it
- Oxygen (O_2): Produced by photosynthesis
- Ozone (O_3): Protects surface from UV radiation
- Methane (CH_4): Potential biological origin

Why Speed Matters:

- Prioritize targets for detailed follow-up
- Rapid assessment of potentially habitable worlds
- Enable systematic surveys of planetary populations