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An Optimal Estimation Spectral Retrieval Approach for Exoplanet Atmospheres

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Abstract

Spectroscopy of exoplanet atmospheres has the potential to provide a wealth of information on their atmospheric properties such as temperature and composition. Here we present a non-linear optimal estimation approach to retrieving exoplanet atmosphere properties from their spectra through a cost function minimization based on the techniques pioneered by [1]. With these tools we can determine the information content and the degrees of freedom for a given spectra and in turn determine, realistically, how much information in terms of temperature and composition can be obtained. We apply these techniques to the well-studied atmospheres of HD189733b, HD209458b, and G436b.

1. Introduction

Madhusudhan & Seager (2009) [2] were the first to pioneer a robust technique to derive temperature and composition of exoplanet atmospheres from fitting the observed spectra. Their technique used ~10 free parameters and an ensemble of $\sim10^7$ forward radiative transfer models of which the best were chosen based off of the minimum chi-squared. Their exhaustive search method did not explore the information content, that is, how much information can be obtained from the observations and how best to obtain it.

We present an alternative approach that can determine the temperature structure and abundances through a cost function minimization.

2. Methods

Following the Rodgers et al. (2000) Bayesian approach, the "best-fit" is obtained when the posterior probability distribution function is maximized, or the cost function is minimized (Eq 1). The state vector values can be retrieved by minimizing this cost function combined with the Levenberg-Marquardt iteration scheme.

Our primary goal is to retrieve the temperature profiles and mixing ratios of H_2O, CO_2, CO, & CH_4 from the spectra. The large error bars and low resolution in transit spectra make it difficult to legitimately retrieve vertical information. Therefore we assume mixing ratio profiles that are constant with altitude for the 4 gases in our model. This is a reasonable assumption due to vertical quenching in these atmospheres [3],[4],[5]. Additionally we parameterize the temperature profile using the two opacity analytical solution from [6]. This provides two additional parameters or a total of 6 parameters to retrieve. We use the Reference Forward radiative transfer Model (RFM—http://www.atm.ox.ac.uk/RFM/) as our forward model, $F(\mathbf{x})$, and include H_2-H_2, H_2-He CIA from [7], CO, CO_2, and H_2O from HITEMP [8] and CH_4 from HITRAN08 [9], given no reliable high temperature (>1000K) CH_4 line list exists (L. Brown private comm.)

With these tools in hand we can calculate the number of degrees of freedom (Eq 2). The number of degrees of freedom tells us realistically, how many pieces of information can be obtained from the data. As a preliminary example, we retrieve the abundances and temperature profiles for HD189733b via the HST NICMOS spectrum [10]. The retrieval typically converges after 4 iterations (Fig 1). We find that the retrieved values of the abundances and temperature profile are similar those found by [2]. We also determine the number of degrees of freedom to be ~4.5, meaning we can successfully retrieve about 4 to 5 parameters. By studying the averaging kernel we can see that most of the information is in the two opacities that govern the temperature profile, and the CO_2 and H_2O mixing ratios. CH_4 and CO are less constrained. In order to address the degeneracy issues an ensemble of retrievals with different *a priori's* must be calculated.

3. Figures

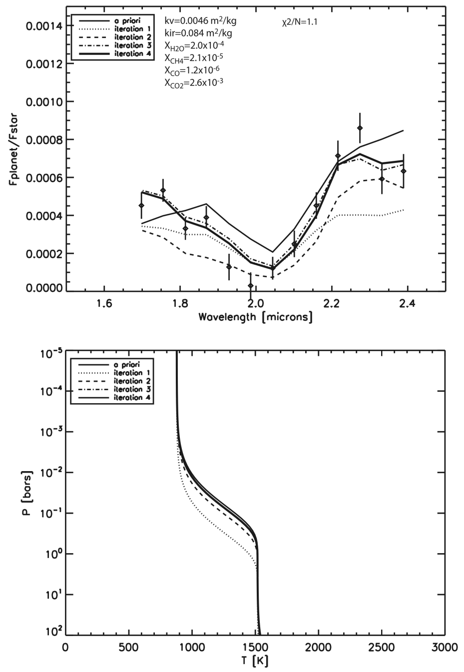

Figure 1. Top: Retrieved model spectra for each iteration. The retrieved visible and infrared opacities along with the constant-with-altitude mixing ratios are given. The reduced χ^2 for the final iteration is also given. Bottom: The temperature profiles corresponding to each iteration. Note that the spectrum is not sensitive to pressure levels higher than ~10 bars and less than ~1 mbar.

4. Equations

$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x}_a)^T \mathbf{S}_a^{-1}(\mathbf{x} - \mathbf{x}_a) + (\mathbf{y} - \mathbf{Kx})^T \mathbf{S}_\varepsilon^{-1}(\mathbf{y} - \mathbf{Kx}) \tag{1}$$

$$d_s = trace(\mathbf{A}) = trace((\mathbf{K}^T\mathbf{S}_\varepsilon^{-1}\mathbf{K} + \mathbf{S}_a^{-1})\mathbf{K}^T\mathbf{S}_\varepsilon^{-1}\mathbf{K}) \tag{2}$$

x=State vector of retrieval variables
y=vector of observations—fluxes vs. wavelength
$\mathbf{x_a}$=*a priori* state vector—initial guess
$\mathbf{S_a}$=*a priori* covariance matrix—expected variance
$\mathbf{S}_\varepsilon$=data error covariance matrix
K=The kernel function (also known as the Jacobian) is the Fréchet derivative of the forward model with respect to the state vector. The elements are $K_{jk} = \frac{\partial F_j(\mathbf{x})}{\partial x_k}$,
J(**x**)=cost function
d_s=number of degrees of freedom
A=averaging kernel—where information is distributed

5. Summary and Conclusions

We have developed a novel approach for retrieving exoplanet atmospheric properties from their spectra based off [1]. This technique can be used to determine how much atmospheric information can be extracted from exoplanet spectra and where that information is distributed. Furthermore, this technique can be used to guide future observations by identifying which channels/wavelengths contain the most useful information about the temperature structure and molecular abundances.

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