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Application of principal component analysis to high spectral resolution radiative transfer: A case study of the O_2 A band

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Abstract

Radiative transfer computation is the rate-limiting step in most high spectral resolution remote sensing retrieval applications. While several techniques have been proposed to speed up radiative transfer calculations, they all suffer from accuracy considerations. We propose a new method, based on a principal component analysis of the optical properties of the system, that addresses these concerns. Taking atmospheric transmission in the $O_2 A$ band as a test case, we reproduced the reflectance spectrum at the top of the atmosphere (TOA), obtained using the multiple scattering code DISORT, with an accuracy of 0.3%, while achieving an order of magnitude improvement in speed.

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1. Introduction

It is well known that the computation of radiative transfer is the bottleneck in remote sensing retrieval problems. The timely retrieval of atmospheric trace gas concentrations from space-borne spectral measurements of radiation reflected through the earth's atmosphere [1] requires computationally efficient sampling techniques in order to accurately model the spectral absorption and scattering signatures of the gases under study.

The first applications of spectral sampling techniques to atmospheric modeling date back to the 1930s (see [2] for an historical account). Since then such techniques have been improved a great deal. A popular scheme is the k-distribution method, which involves grouping spectral intervals according to absorption coefficient (k) strength ([3–7]). An extension of this method is the correlated k-distribution method, by which the frequency order of absorption coefficients for one gas rearranged by strength at one altitude is the same as that at another ([8–12]).

The drawback of the correlated k-distribution method is that it assumes that atmospheric optical properties are spectrally correlated at all points along the optical path, such that spectral intervals with similar optical properties at one level of the atmosphere will remain similar at all other levels. This assumption is rigorously valid for homogeneous, isobaric, isothermal optical paths, but it usually breaks down for realistic inhomogeneous, non-isothermal, atmospheric optical paths. This loss of correlation can sometimes introduce significant radiance errors.

Spectral mapping methods [13,14] have also been proposed to enhance computational speed. Like the correlated k-distribution method, spectral mapping methods gain their efficiency by identifying spectral intervals that have similar optical properties. These intervals are then gathered into bins, and a single monochromatic multiple scattering calculation can be performed for each bin. Spectral mapping methods make no assumptions about the spectral correlation along the optical path. Instead, these methods perform a level-by-level comparison of monochromatic atmospheric and surface optical properties, and combine only those spectral regions that actually remain in agreement at all points along the inhomogeneous optical path. The disadvantage here is that fine spectral binning is required to maintain accuracy in the radiative transfer calculation, but this results in minimal gains in computational efficiency and comes at the expense of a significantly more complex retrieval code. Coarse spectral binning, on the other hand, provides excellent computational efficiency increases at the expense of significant reduction in the accuracy of the calculated radiances. Also, since different bins are used for the calculation, there are discontinuities in the partial derivatives.

Thus, there is clearly a need for an alternative scheme that does not compromise on accuracy while enhancing computational efficiency.

2. Model description

In our analysis, we seek an accurate and efficient characterization of near-infrared (NIR) absorption in the O₂ A band centered at 760 nm. O₂ A band observations can provide surface pressure estimates with accuracies of $\sim 1 \text{ mbar [15]}$. The presence of strong and weak absorption lines also makes it useful for characterizing the vertical distribution of clouds and aerosols [16].

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