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Linearization of the Principal Component Analysis method for radiative transfer acceleration: Application to retrieval algorithms and sensitivity studies

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ABSTRACT

Principal Component Analysis (PCA) is a promising tool for enhancing radiative transfer (RT) performance. When applied to binned optical property data sets, PCA exploits redundancy in the optical data, and restricts the number of full multiple-scatter calculations to those optical states corresponding to the most important principal components, yet still maintaining high accuracy in the radiance approximations. We show that the entire PCA RT enhancement process is analytically differentiable with respect to any atmospheric or surface parameter, thus allowing for accurate and fast approximations of Jacobian matrices, in addition to radiances. This linearization greatly extends the power and scope of the PCA method to many remote sensing retrieval applications and sensitivity studies. In the first example, we examine accuracy for PCA-derived UV-backscatter radiance and Jacobian fields over a 290–340 nm window. In a second application, we show that performance for UV-based total ozone column retrieval is considerably improved without compromising the accuracy.

1. Introduction

Radiative transfer (RT) modeling is an essential component of remote sensing retrieval. RT models are required for the generation of simulated radiances from satellite, ground-based and other platforms. In many inverse-modeling applications, the RT models are also needed to calculate Jacobians (partial derivatives of radiances with respect to atmospheric, surface or other parameters). RT calculations are expensive from the computational viewpoint; this is especially the case in the solar scattering regime, where full multiple-scattering computations are often needed for many spectral points.

In recent years, there have been a number of developments for Observation System Simulation Experiments (OSSEs); these experiments are often designed to investigate possible strategies for instrument synergy, and they invariably require massive RT forward modeling over wide spectral ranges. Furthermore, new-generation low-orbit and geostationary satellite instruments coming up for launch in the next decade will be generating data at rates that current computing power is unlikely to match. For example, the TROPOMI instrument [1] on the Sentinel-5 Precursor (2015 launch) is expected to produce about one order of magnitude more data than its predecessor OMI (launched in 2004), and about 50 times more data than GOME-2 on MetOp-A and MetOp-B (launched 2006 and 2012) [2]. For these and other reasons, there is a pressing need for RT performance enhancement for a wide range of applications.

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Over the years, there have been many attempts to enhance performance of RT modeling; these include correlated-k methods [3], spectral binning [4,5], asymptotic methods for semi-infinite media (see [6] for a review), Principal Component Analysis (PCA), use of low-stream interpolation methods [7,8], low-orders of scattering approximations [9] and neural networks (e.g. [10]). A comprehensive review of RT performance enhancement methods has appeared in a recent paper [11]. In contrast to these software acceleration techniques, we note that hardware methods (GPU cards) have started to make an impact; see for example [12].

PCA is a mathematical transformation that converts a correlated mean-subtracted data set into a series of 'principal components' (PCs). The transformation is orthogonal: the first PC accounts for the largest variance in the original data, with subsequent PCs accounting for the remainder of the data variance, each PC being uncorrelated with the others. PCA is also known as the method of Empirical Orthogonal Functions (EOFs); for a review see [13]. PCA gives insight into variability patterns in data sets, and is important in data compression; the first few PCs will typically capture almost all the variance if there is significant correlation in the original data. In stochastic processes, PCA is known as the Karhunen–Loève transform, or the Hotelling transform. In geophysics applications, PCA is performed by eigenvalue methods or singular-value decomposition techniques.

In the PCA application for RT performance enhancement, EOFs are developed for spectrally-binned sets of inherent optical properties which possess some redundancy; costly multiple-scattering RT calculations are only done for a few EOF-derived optical states, and from these calculations, correction factors are applied to approximately-calculated radiation fields computed with fast RT models. This PCA technique was first applied to scalar radiance simulations (no polarization) at high resolution in and around the O_2 A band [14], and later expanded to RT modeling with polarization for the O_2 A band and the weak and strong CO_2 absorptions bands (1.61 μm, 2.03 μm) [15]. The latter work was done in the context of remote sensing of CO_2 by the OCO platform [16].

The present work is the first of a series of papers extending the PCA method to a much wider set of applications in remote sensing and the field of Observing System Simulation Experiments (OSSEs). We present a number of new theoretical developments, mainly concerning the analytic linearization of the PCA procedure itself, and the subsequent development of analytic Jacobians for the PCA-based radiation fields. This first paper is confined to scalar RT simulations in the solar UV-backscatter regime. The second paper in this series will deal with RT applications in the thermal emission and cross-over (emission plus scattering) regimes; the third paper will examine PCA performance enhancement for linearized vector RT applications, and a fourth paper will look at effects from bidirectionally reflecting surfaces.

In Section 2, we present the PCA theory for RT performance enhancement, and describe new derivations for the analytic treatment of weighting functions in the PCA context. In Section 3, we summarize the RT models used in this study. Section 4 contains two examples from UV backscatter modeling appropriate to past and present nadir-viewing atmospheric chemistry instruments such as GOME, GOME-2, SCIAMACHY and OMI, and future instruments such as TROPOMI and Sentinel 4 and 5. In Section 4.1, we look at PCA-derived calculations of radiances and total-ozone Jacobians over the 290–340 nm range, and in Section 4.2 we examine performance enhancement for the direct-fitting retrieval of total ozone in the 325–335 nm window.

2. Fast RT modeling with PCA

2.1. General formulation

We assume an atmosphere stratified into a set of optically uniform layers. For each layer n ($n=1\ldots N$) and each spectral point i in a wavelength window with S such values, we define layer extinction optical thickness values τ_{ni}, total single scattering albedos ω_{ni}, and phase function expansion coefficients β_{nli}, such that the phase function $\Pi_{ni}(\Theta) = \Sigma_l \beta_{nli} P_l(\cos\Theta)$ is expressed in terms of Legendre polynomials $P_l(\cos\Theta)$ in the cosine of the scattering angle Θ. The optical states $\{\tau_{ni}, \omega_{ni}, \beta_{nli}\}$ comprise the *inherent optical properties* of the atmosphere required as input to the RT models.

In an atmosphere with trace gas absorption, molecular scattering and aerosol extinction and scattering, we can express these optical properties in terms of trace gas absorption optical thicknesses γ_{ni}, molecular scattering thickness values ρ_{ni}, and aerosol extinction and scattering optical thicknesses ϵ_{ni} and κ_{ni} respectively, through the relations:

$$\tau_{ni} = \gamma_{ni} + \rho_{ni} + \varepsilon_{ni}; \quad \omega_{ni} = \frac{\rho_{ni} + \kappa_{ni}}{\tau_{ni}};$$

$$\beta_{nli} = \frac{\rho_{ni}\beta_{nli}^{(Ray)} + \kappa_{ni}\beta_{nli}^{(Aer)}}{\rho_{ni} + \kappa_{ni}}. \qquad (1)$$

Here, $\beta_{nli}^{(Ray)}$ and $\beta_{nli}^{(Aer)}$ are the phase function expansion coefficients for the molecular and aerosol phase functions respectively. In a pure Rayleigh atmosphere, we have $\tau_{ni} = \gamma_{ni} + \tau_{ni}\omega_{ni}$. Total-atmosphere optical depths may be denoted for example by $T_i = \Sigma_n \tau_{ni}$ and $\Gamma_i = \Sigma_n \gamma_{ni}$ for extinction and trace-gas absorption respectively.

Fig. 1 is a visualization of the data set $\{\tau_{ni}, \omega_{ni}\}$ for a 13-layer atmosphere with Rayleigh scattering and ozone absorption in the UV. There are 88 spectral points in the window 325–335 nm. [We will encounter this data set again in Section 4.2]

The main goal of the work is to speed up the performance of radiative transfer modeling for hyper-spectral applications. For a window with thousands of spectral points, there is invariably a large dynamic range of optical depths, and it will be necessary to partition the window into a number of spectral bins. Each bin is characterized by grouping certain optical properties (such as atmospheric layer optical thickness values or single scattering albedos) that are similar within the bin. The selection for spectral binning is often based on the division of (the logarithms of) the total-atmosphere optical depths T_i or Γ_i into decadal intervals (see for example [15]). We discuss the binning in more detail below, and again for the case studies in Section 4.