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Optical property dimensionality reduction techniques for accelerated radiative transfer performance: Application to remote sensing total ozone retrievals

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ABSTRACT

In this paper, we introduce several dimensionality reduction techniques for optical parameters. We consider the principal component analysis, the local linear embedding methods (locality pursuit embedding, locality preserving projection, locally embedded analysis), and discrete orthogonal transforms (cosine, Legendre, wavelet). The principle component analysis has already been shown to be an effective and accurate method of enhancing radiative transfer performance for simulations in an absorbing and a scattering atmosphere. By linearizing the corresponding radiative transfer model, we analyze the applicability of the proposed methods to a practical problem of total ozone column retrieval from UV-backscatter measurements.

1. Introduction

The new generation of infrared satellite instruments provides high spatial and spectral resolution spectra. There are two ways to process and analyze efficiently the hyperspectral information from these instruments [1]. The first option is to reduce the computational time of the radiative transfer calculations. The correlated k distribution [2], the exponential sum fitting transmittance [3], the radiance sampling method [4], and the optimal spectral mapping method [5] are examples of fast radiative transfer models. The second option is to perform an optimal inversion of the measured spectra by using dimensionality reduction techniques [6,7]. More precisely, the principal component analysis (PCA) is used to map the spectral radiances into a lower-dimensional subspace, in which the inversion is performed.

Massive amounts of spectral information will be generated by the new generation of European atmospheric sensors Sentinel 5 Precursor, Sentinel 4 and Sentinel 5. A fast processing of the data in the UV–VIS spectral domain is required. Several techniques have been proposed to deal with this problem. In the operational processor for the SCIAMACHY instrument, the radiance at the wavelength λ is computed as

$$\ln \frac{I(\lambda,\boldsymbol{\xi})}{I_a(\lambda,\boldsymbol{\xi})} = f_{\mathrm{I}}(\lambda,\boldsymbol{\xi}), \tag{1}$$

where $\boldsymbol{\xi}$ is the vector of atmospheric parameters to be retrieved, I_a is the radiance computed by an approximate radiative transfer model, e.g., a two-stream or a single scattering model, and f_{I} is a correction factor [8]. For efficiency reasons, the correction factor is computed at the initial guess $\boldsymbol{\xi}_0$, and is kept constant during the retrieval, i.e., $f_{\mathrm{I}}(\lambda,\boldsymbol{\xi}) = f_{\mathrm{I}}(\lambda,\boldsymbol{\xi}_0)$. An improved approximation is $f_{\mathrm{I}}(\lambda,\boldsymbol{\xi}) = P_{\xi}(\lambda) f_{\mathrm{I}}(\lambda,\boldsymbol{\xi}_0) + Q_{\xi}(\lambda)$, with P_{ξ} and Q_{ξ} being low-order polynomials in wavelength. The coefficients of the polynomials are computed at each iteration step by minimizing the residuals based on Eq. (1) as a forward model at a reduced set of discrete wavelengths. This technique

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suffers from a low accuracy of the computed radiances, especially for a cloudy atmosphere.

A very efficient and an accurate method for computing the radiance correction factor has been given by Natraj et al. [9,10]. This approach, which increases the computational efficiency of radiative transfer calculations in an absorbing and a scattering atmosphere, has the following attributes:

1. The approximate model is a two-stream radiative transfer model, while the reference model is a multi-stream radiative transfer model.
2. The PCA is used to reduce the dimensionality of the optical parameters of the atmospheric system.
3. The dependency of the correction factor on the optical parameters is modeled by a second-order Taylor expansion about the mean value of the optical parameters.

The performance of this method is remarkable; for example, the oxygen A-band spectrum was reproduced with an accuracy of 0.3%, while achieving an order of magnitude speed improvement. A linearized version of this PCA-based radiative transfer model and its application to the direct fitting of total ozone columns from GOME-type sensors have been provided by Spurr et al. [11]. The authors found that the accuracy of the results is better than 0.5% when 2 or more empirical orthogonal functions are used, and that the performance enhancement is of about 3.5–4 for 4 discrete ordinates in the polar hemisphere.

The goal of this paper is to demonstrate the powerfulness and the flexibility of the PCA-based radiative transfer model described in [9,10]. For this purpose, we formulate the dimensionality reduction problem of the optical parameters in a general framework, and design a linearized radiative transfer model in this setting. Then, we introduce several dimensionality reduction techniques including linear embedding methods and discrete orthogonal transforms. Finally, we analyze the accuracy and the efficiency of these methods by retrieving total ozone column from Global Ozone Monitoring Experiment (GOME) measurements.

2. Radiative transfer model based on dimensionality reduction methods

Let us consider an atmospheric scenario consisting of trace gases and a homogeneous cloud layer, and let us assume that the cloud extinction and scattering coefficients, as well as the cloud phase function, are constant within the spectral retrieval interval. As a result, the wavelength-dependent parameters are the trace gas absorption coefficient $\sigma^{\mathrm{gas}}_{\mathrm{abs}}(\lambda,z)$, the scattering coefficient of air molecules $\sigma^{\mathrm{mol}}_{\mathrm{sct}}(\lambda,z)$, the Rayleigh scattering phase function $P_{\mathrm{Ray}}(\lambda,z)$, and the surface albedo $A(\lambda)$. Assuming further that the Rayleigh scattering phase function does not vary significantly within the considered spectral interval, and considering a discretization of the atmosphere in L layers, we define, as in [9–11], an N-dimensional vector $\mathbf{x}_w$, for each wavelength λ_w, by

$$\mathbf{x}_w^T = [\ln \sigma^{\mathrm{gas}}_{\mathrm{abs}1}(\lambda_w),\ldots,\ln \sigma^{\mathrm{gas}}_{\mathrm{abs}L}(\lambda_w),\ln \sigma^{\mathrm{mol}}_{\mathrm{sct}1}(\lambda_w),\ldots,\ln \sigma^{\mathrm{mol}}_{\mathrm{sct}L}(\lambda_w),\ln A(\lambda_w)], \tag{2}$$

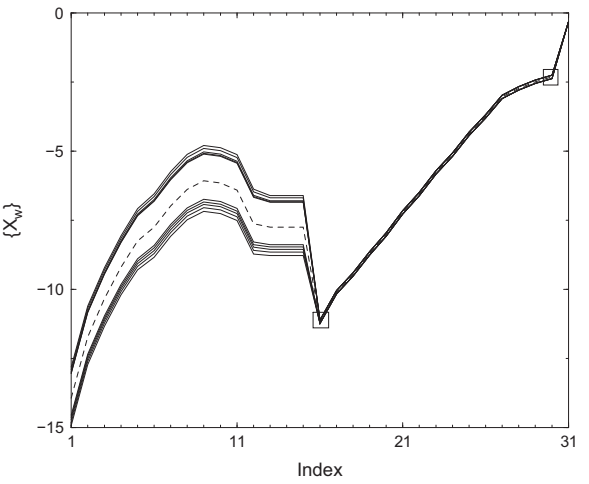

Fig. 1. Some vectors $\mathbf{x}_w$ for the ozone retrieval problem considered in Section 5. The different continuous curves correspond to different wavelengths in the spectral interval 325–335 nm, while the dashed curve corresponds to the sample mean. The boxes mark the discontinuities in the entries of $\mathbf{x}_w$, when passing from the vector of trace gas absorption coefficients (entries from 1 to 15) to the vector of scattering coefficients (entries from 16 to 30), and from the latter to the surface albedo.

where $\sigma^{\mathrm{gas}}_{\mathrm{abs}k}(\mathrm{km}^{-1})$ and $\sigma^{\mathrm{mol}}_{\mathrm{sct}k}(\mathrm{km}^{-1})$ are the optical coefficients in the kth layer, and $N=2L+1$. Thus, the wavelength variability of the optical parameters, representing the input parameters of the radiative transfer code, is encapsulated in the vector $\mathbf{x_w}$. By this construction we have established a one-to-one correspondence between the discrete set of all wavelengths of interest $\{\lambda_w\}_{w=1}^{W}$ and the discrete set of optical parameters $\{\mathbf{x}_w\}_{w=1}^{W}$, where W is the number of spectral points. Note that usually $N<W$. In Fig. 1 we illustrate the first five and the last five vectors $\mathbf{x}_w$ for the ozone retrieval problem considered in Section 5 and corresponding to $W=88$ and $L=15$. It is clear from this figure that the variability of the scattering coefficient is much lower than that of the trace gas absorption coefficient.

High-dimensional real data often lies on or near a lower-dimensional manifold. The fundamental issues in dimensionality reduction are the modeling of the geometry structure of the manifold, and the design of an appropriate embedding for data projection. For the N-dimensional data set $\{\mathbf{x}_w\}_{w=1}^{W}$, where $\mathbf{x}_w\in\mathbb{R}^N$, let $\overline{\mathbf{x}}=(1/W)\sum_{w=1}^{W}\mathbf{x}_w$ be the sample mean of the data. The goal of a linear embedding method is to find an M-dimensional subspace ($M<N<W$) spanned by a set of linear independent vectors $\{\mathbf{a}_k\}_{k=1}^{M}$, such that the centered (mean-removed) data $\mathbf{x}_w-\overline{\mathbf{x}}$ lie mainly on this subspace (manifold),

$$\mathbf{x}_w \approx \overline{\mathbf{x}} + \sum_{k=1}^{M} y_{wk}\mathbf{a}_k = \overline{\mathbf{x}} + \mathbf{A}\mathbf{y}_w, \quad w=1,\ldots,W, \tag{3}$$

here $\mathbf{A}:=[\mathbf{a}_k]_{k=1}^{M}$ is an $N\times M$ matrix comprising the column vectors $\mathbf{a}_k$ and y_{wk} is the kth component of the vector of parameters $\mathbf{y}_w\in\mathbb{R}^M$. In the dimensionality reduction theory, the matrix $\mathbf{A}$ represents the (inverse) mapping from the low-dimensional space to the high-dimensional space. The vector of parameters $\mathbf{y}_w$ is given by the forward mapping from the high-dimensional space to the low-dimensional