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Calculation of Jacobians for inverse radiative transfer: An efficient hybrid method

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Abstract

We present an accurate and numerically efficient procedure of calculating Jacobians by finite difference that consists of two components: (1) a method employing the saving of atmospheric layers that accelerates the solution to the equation of radiative transfer for solvers that use the Discrete Space formulation and (2) a method of perturbing the eigenmatrix spectrum associated with a reduced attenuation matrix. The procedure eliminates the need to call the eigenmatrix package, here, LAPACK a second time and provides insights into the fundamental properties of the attenuation matrix, useful for characterizing the accuracy of the derivatives calculated by finite difference methods. The computational complexity of the perturbation method is $8n^3 + 22n^2$, where n is one half the number of streams in the radiance field as opposed to $16n^3$ using LAPACK. The method is not limited to the calculation of base state radiances $I(\omega)$ and those associated with an 'infinitesimal' perturbation $I(\omega + \delta\omega)$ (from which the numerical derivative of $I(\omega + \delta\omega)$ with respect to $\delta\omega$ may be approximated), but is also useful in the calculation of radiances associated with a 'finite' perturbation $I(\omega + \Delta\omega)$ from which a sensitivity can be calculated.

Keywords: Jacobians; Perturbations

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1. Introduction

Many remote sensing methods that provide inferences of optical or physical properties of the system being observed require the inversion of various forms of the radiative transfer equation (RTE). This inversion takes several forms, and the more complex radiative transfer (RT) problems most often adopt some form of iterative, non-linear optimal estimation scheme (e.g. Rogers [1]). In this framework, inversion requires the evaluation of Jacobians (i.e., a matrix containing the derivatives of the radiances with respect to the quantities sought). In atmospheric applications, this frequently requires evaluation at many wavelengths and many layers. Because the potential dimensionality of this problem is high, it is important to develop computationally efficient methods for deriving these Jacobians.

In response to this need, this paper describes computationally efficient methods of calculating the derivatives of the radiances with respect to the optical properties for the RT problem involving multiple scattering, absorption and emission. A simple approach to calculating the Jacobian is to solve the RTE twice: one call to compute the radiance for a base state defined by the profile of an atmospheric constituent and a second call to a final state that is the same as the base state but in which the value of a constituent in a layer has been perturbed. If the change in the optical properties is sufficiently small, the difference between the calculated radiance of the perturbed and base state divided by the size of the perturbation approximates the required derivative. Unless the RTE is sufficiently simple, as would be the case in the absence of scattering or in optically thin media, calling the RT solver twice as required in forward or backward differencing, or three times, as in central differencing imposes high computational cost.

In the case of pure absorption, analytical Jacobians exist (e.g. [2,3]). When multiple scattering is important, a few codes have also been developed to compute Jacobians. These codes fall into two broad catagories: those developed for use with atmospheres of small optical depths and those applicable to atmospheres of arbitrary optical depth. Examples of the former are GOMETRAN [4] and LIRA [5]. An example of the latter is LIDORT [6]. These codes have two features in common: (1) they perturb a base state optical property to compute corrections to the base state radiances and (2) corrections to the base state radiances are first order accurate with respect to the perturbed parameter of interest. A later version of LIDORT [7] is a truly analytical code in that it does not require any perturbations to be specified by the user and is also available. This is a general purpose code whose analycity derives from the requirement that the user enter partial derivatives of optical properties with respect to the physical variables of interest. It follows that all of the aforementioned codes can compute final state radiances from those of the base state provided that the radiances change linearly within the range of the perturbation; otherwise, local curvature may introduce significant error. In this paper we show how the introduction of higher order corrections can be accommodated by perturbing the eigenspectrum. The method, applicable to the discrete space formulation [8] of solving the RTE is hereafter referred to as the spectral perturbation method. The implementation is straightforward, numerically stable, and for small changes in optical properties, extremely accurate and efficient over a tested span in optical properties that is likely to be encountered in the real atmosphere. The method also yields insights into the numerical properties of the attenuation matrix, fundamental to the solution method described here and in DISORT [9]. Also, a simple procedure called layer-saving is presented which reduces the number of calculations in a multi-layered atmosphere by compositing and saving all