

On the generation of atmospheric-property Jacobians from the LIDORT linearized RT models

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Abstract

The linearized radiative transfer models VLIDORT and LIDORT will deliver profile weighting functions (Jacobians) with respect to layer optical properties. We derive transformation rules for the conversion of layer Jacobian output to weighting functions defined for level (layer boundary) quantities such as volume mixing ratio, temperature and pressure. In a related development, we discuss the derivation of bulk-property atmospheric Jacobians with respect to quantities such as the temperature shift, the surface pressure and scaling parameters for constituent profiles. We also present some rules for calculating Jacobians for parameters characterizing aerosol loading regimes. An appendix contains linearization (with respect to temperature and pressure) of the trace species cross-sections derived from the HITRAN line spectroscopy data base.

Keywords: Radiative transfer; Jacobian transformation rules; cross-section derivatives.

1. Introduction

Remote sensing retrievals of atmospheric profile properties (pressure, temperature) and constituents (trace gas amounts, aerosol loadings) are usually implemented using classical inverse methods based on cost-function minimization between measured and simulated satellite radiances [1]. In the solar regime, these retrievals require the use of a linearized forward model that is

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based on an accurate radiative transfer (RT) treatment of light scattering and extinction. The RT model must generate not only simulated radiances but also all necessary profile weighting functions (Jacobians) - these are partial derivatives of the intensity field with respect to profiles of pressure, temperature and constituent amounts.

For computational convenience using 1-D RT models, the atmosphere is discretized into a number of stratifications, each layer being treated as optically uniform. A general scattering code such as DISORT [2] or (V)LIDORT [3] or DOME [4] will then require as input the specification of a complete set of optical properties defined for each such layer - the total extinction optical depths, the total single scattering albedos, and the total phase function or scattering matrix in each layer. Most scalar RT models are based on expansions of the phase function in terms of Legendre polynomials, and it is then sufficient to specify the set of expansion coefficients. For most vector RT simulations (with polarization), elements of the scattering matrix are expanded in terms of generalized spherical functions with associated sets of coefficients.

If the RT model is linearized, it is then possible to generate Jacobians or weighting functions with respect to these optical property inputs. For instance the LIDORT (scalar) and VLIDORT (vector) discrete ordinate models are analytically differentiable with respect to their layer optical inputs. Jacobians obtained in this manner are layer quantities. Jacobians with respect to layer profile quantities such as ozone Umkehr columns or layer aerosol optical depths may be obtained directly from LIDORT.

However, layer optical properties are mostly constructed from atmospheric quantities specified at various *levels* in the atmosphere; it is often the case that these levels actually define the stratification to be used in the RT calculations. Aside from the scattering expansion coefficients, layer optical quantities are obtained by integration of optical densities between the two level boundaries. In this regard, air and gas particle densities are dependent on temperature and pressure, as are absorption cross-sections.

The question of interest here is to define RT Jacobians with respect to *level* atmospheric properties (pressure temperature, volume mixing ratios (VMRs), aerosol concentrations), given a set of relations expressing layer optical properties in terms of these level quantities. Such a process will require the use of chain-rule differentiation based on a set of “layers-to-levels” transformations inherent in the manner in which the optical properties are constructed. This issue has been examined in detail for thermal emission RT

in the absence of scattering - see for example [5] . In the present note, we discuss this “layers-to-levels” Jacobians for a scattering RT scenario.

The second topic in this note concerns the derivation of LIDORT inputs to generate bulk-property Jacobians, that is, weighting functions with respect to whole-atmosphere quantities such as temperature shift, scaling factors for VMR profiles, surface pressure, total amounts of trace species or total aerosol optical depths. We show how to set up these inputs given atmospheric profiles specified at levels.

Also in this regard, we examine the specification of aerosol profiles in terms of simple functions characterized by small sets of defining parameters such as the total loading, the relaxation constant for an exponential decay profile, or the peak height for a Gaussian-type profile. We then derive rules for setting up LIDORT Jacobians with respect to these parameters.

The scope of this note is straightforward. In section 2, we deal with the level-output profile Jacobian specification. We obtain rules for converting LIDORT optical-layer Jacobian output to level-atmosphere weighting functions, and we examine the use of fine-layering schemes when carrying out the layers to levels transformations. Section 3 is concerned with bulk property Jacobians for temperature-shift and related quantities, and for aerosol loading parameterizations. Section 4 has some concluding remarks on applications, and the appendix has a discussion on the derivation of analytic derivatives of line-spectroscopic cross-sections with respect to temperature and pressure.

2. Jacobians: Optical-layer to Level-atmosphere Output

2.1. LIDORT Jacobians based on layer optical properties

LIDORT is a stratified multi-layer radiative transfer model that requires as input a set of optical properties $\{\Delta_n, \omega_n, \beta_{n,l}\}$ defined for each layer n . The total optical thickness Δ_n , total single scattering albedo ω_n and total phase function expansion coefficients $\beta_{n,l}$ are given by

$$\Delta_n = G_n + R_n + A_n \quad (1)$$

$$\omega_n = \frac{R_n + z_n A_n}{\Delta_n} \quad (2)$$

$$\beta_{n,l} = \frac{R_n \beta_l^{Ray} + z_n A_n \beta_{n,l}^{Aer}}{R_n + z_n A_n} \quad (3)$$

where G_n is the molecular (trace gas) absorption optical depth, R_n the molecular (Rayleigh) scattering optical depth, A_n the aerosol extinction optical depth, z_n the aerosol single scattering albedo, β_l^{Ray} the Rayleigh scattering phase function Legendre expansion coefficients, and $\beta_{n,l}^{Aer}$ the aerosol phase function expansion coefficients.

In order that LIDORT can deliver *layer* profile Jacobians

$$\frac{\partial I}{\partial G_n}, \frac{\partial I}{\partial R_n}, \frac{\partial I}{\partial A_n} \quad (4)$$

with respect to the three optical depth quantities, we must generate additional LIDORT inputs, which are the following group of linearized optical properties, derived by simple differentiation of the above equations

$$\frac{\partial \Delta_n}{\partial G_n} = 1; \quad \frac{\partial \omega_n}{\partial G_n} = -\frac{\omega_n}{\Delta_n}; \quad \frac{\partial \beta_{n,l}}{\partial G_n} = 0. \quad (5)$$

$$\frac{\partial \Delta_n}{\partial R_n} = 1; \quad \frac{\partial \omega_n}{\partial R_n} = -\frac{(1 - \omega_n)}{\Delta_n}; \quad \frac{\partial \beta_{n,l}}{\partial R_n} = \frac{(\beta_l^{Ray} - \beta_{n,l})}{R_n + z_n A_n}. \quad (6)$$

$$\frac{\partial \Delta_n}{\partial A_n} = 1; \quad \frac{\partial \omega_n}{\partial A_n} = -\frac{(z_n - \omega_n)}{\Delta_n}; \quad \frac{\partial \beta_{n,l}}{\partial A_n} = \frac{(z_n \beta_{n,l}^{Aer} - \beta_{n,l})}{R_n + z_n A_n}. \quad (7)$$

The procedure for VLIDORT is very similar, except that we are now dealing with Stokes 4-vectors $\mathbf{I} = [I, Q, U, V]^T$ appropriate to polarized-light RT instead of scalar intensity I , and the scalar phase function expansion coefficients are replaced by sets of 6 coefficients corresponding to generalized spherical function expansions of the scattering matrix [3].

2.2. Formulation of the problem

The problem may be stated very simply: Given profile Jacobian output from (V)LIDORT with respect to *optical* properties in *layers*, how do we derive profile Jacobian output with respect to *atmospheric* properties defined on *levels* (layer boundaries)?

In order to answer this question, we make several assumptions.

- 1) Atmospheric quantities (pressure, temperature, height, trace gas volume mixing ratios, aerosol particle concentrations) are defined at levels (layer boundaries) and all level quantities (except height) are regarded as independent variables with respect to which "level" Jacobians of the radiance field are defined.

- 2) For pressure, temperature and height, the atmosphere may be prepared in hydrostatic equilibrium, and the air density at each level is proportional to the pressure and to the inverse of the temperature, the constant of proportionality expressed in terms of the density at standard temperature and pressure (STP).
- 3) For aerosols, the number concentration profile depends only on the height; optical properties are constant.
- 4) Integration between levels will be done using simple trapezoidal summation, with or without a fine-layering scheme, and with temperatures and logarithmic pressures interpolating linearly with level boundary heights.

Assumption (1) postulates a set of variables $\{p_n, T_n, h_n, v_n, x_n\}$ (pressure, temperature, height, volume mixing ratio and aerosol concentration respectively), defined at levels $n = 0, \dots, N$, with the convention that the top of the atmosphere is at level 0, level 1 is the bottom of layer 1, etc., and Level N is the lower (surface) boundary. Further, the associated Jacobians $\partial I / \partial T_n$, $\partial I / \partial P_n$, $\partial I / \partial v_n$, and $\partial I / \partial x_n$ are all defined.

Assumption (2) states that the air density at level n is given by $\rho_n = C \frac{p_n}{T_n}$, where C is a constant related to the density at STP, and the trace gas density at this level is then given by $\rho_n v_n$.

2.3. Generation of layer optical properties from level inputs

Without loss of generality, we assume only one trace gas constituent with volume mixing ratio profile $\{v_n\}$ defined at levels n . We will examine derivation of Jacobians with respect to $\{v_n\}$, temperature profile $\{T_n\}$ and aerosol concentration profile $\{x_n\}$. Also, we assume there are no fine-layers in the height integration between levels; fine layering is discussed in the next section.

From assumption (2), it follows that the trace gas optical thickness $G_{j,n}$ in layer n at spectral point j is

$$G_{j,n} = \frac{1}{2} C d_n \left(\frac{v_n p_n \sigma_{j,n}}{T_n} + \frac{v_{n-1} p_{n-1} \sigma_{j,n-1}}{T_{n-1}} \right). \quad (8)$$

Here C is a constant, $d_n = h_{n-1} - h_n$ is the height separation (layer vertical extent), and the cross-sections $\sigma_{j,n}(T_n, p_n)$ are assumed to be known functions of temperature and pressure. We may define the Rayleigh scattering

optical thickness $R_{j,n}$ in a similar way, treating the Rayleigh cross-section ς_j as independent of temperature and pressure:

$$R_{j,n} = \frac{1}{2} C \varsigma_j d_n \left(\frac{p_n}{T_n} + \frac{p_{n-1}}{T_{n-1}} \right). \quad (9)$$

From assumption (3), the aerosol extinction cross-section ϵ_j is independent of temperature and pressure, and the aerosol optical thickness $A_{j,n}$ is then

$$A_{j,n} = \frac{1}{2} \epsilon_j d_n (x_n + x_{n-1}). \quad (10)$$

In order to derive suitable Jacobians, we require the derivatives of these quantities with respect to the defining properties. From Eqs. (8) and (9), we have the following temperature partial derivatives for $k = n - 1$ or $k = n$:

$$\frac{\partial G_{j,n}}{\partial T_k} = \frac{1}{2} C d_n \frac{v_k p_k}{T_k} \left(\frac{\partial \sigma_{j,k}}{\partial T_k} - \frac{\sigma_{j,k}}{T_k} \right); \quad (11)$$

$$\frac{\partial R_{j,n}}{\partial T_k} = -\frac{1}{2} C d_n \frac{p_k \varsigma_j}{T_k^2}. \quad (12)$$

The trace gas VMR derivative is then

$$\frac{\partial G_{j,n}}{\partial v_k} = \frac{1}{2} C d_n \frac{p_k \sigma_{j,k}}{T_k}; \quad (13)$$

Similarly, the aerosol profile derivative is

$$\frac{\partial A_{j,n}}{\partial x_k} = \frac{1}{2} d_n \epsilon_j; \quad (14)$$

Note that this levels-to-layers transformation is not part of LIDORT; the radiative transfer model only deals with layer quantities. Clearly, the transformation depends on the application and the manner by which the atmospheric constituent profiles have been constructed. In particular, it is implicit in our treatment that level pressures and temperatures are independently varying quantities.

An important application in the UV backscatter region concerns ozone profile and column retrievals. In this case, the ozone Huggins band cross-sections have the well known Bass-Paur quadratic temperature parameterization [6]:

$$\sigma_{j,k} = \sigma_j^{(0)} + \sigma_j^{(1)} (T_k - \theta^*) + \sigma_j^{(2)} (T_k - \theta^*)^2. \quad (15)$$

for ozone cross-sections $\sigma_{j,k}$ at spectral point j , where the (level) temperatures are in degrees K and $\theta^* = 273.15K$. Temperature derivatives are easy to write down:

$$\frac{\partial \sigma_{j,k}}{\partial T_k} = \sigma_j^{(1)} + 2\sigma_j^{(2)}(T_k - \theta^*). \quad (16)$$

In the near and short-wave infrared (NIR/SWIR) spectral regions, trace gas absorption cross-sections are derived through line spectroscopic methods, and it is necessary to obtain both temperature and pressure derivatives $\frac{\partial \sigma_{j,k}}{\partial T_k}$ and $\frac{\partial \sigma_{j,k}}{\partial p_k}$ in order to generate the corresponding profile Jacobians. In the Appendix, we discuss the analytic derivation of these cross-section derivatives for Voigt-profile line spectroscopy.

2.4. Transformation rules for level-atmosphere Jacobians

Given the layer Jacobians from LIDORT as defined Eq. (4), we may derive the level VMR Jacobians by using the following chain rule transformation (suppressing the spectral index)

$$\frac{\partial I}{\partial v_0} = \frac{\partial I}{\partial G_1} \cdot \frac{\partial G_1}{\partial v_0}; \quad (17)$$

$$\frac{\partial I}{\partial v_k} = \frac{\partial I}{\partial G_k} \cdot \frac{\partial G_k}{\partial v_k} + \frac{\partial I}{\partial G_{k+1}} \cdot \frac{\partial G_{k+1}}{\partial v_k}, \quad k = 1, \dots, N-1; \quad (18)$$

$$\frac{\partial I}{\partial v_N} = \frac{\partial I}{\partial G_N} \cdot \frac{\partial G_N}{\partial v_N}. \quad (19)$$

We may derive a similar transformation rule for the temperature Jacobians, this time remembering that both the trace gas and Rayleigh scattering optical properties have temperature dependence:

$$\frac{\partial I}{\partial T_0} = \frac{\partial I}{\partial G_1} \cdot \frac{\partial G_1}{\partial T_0} + \frac{\partial I}{\partial R_1} \cdot \frac{\partial R_1}{\partial T_0}; \quad (20)$$

$$\begin{aligned} \frac{\partial I}{\partial T_k} = & \left(\frac{\partial I}{\partial G_k} \cdot \frac{\partial G_k}{\partial T_k} + \frac{\partial I}{\partial G_{k+1}} \cdot \frac{\partial G_{k+1}}{\partial T_k} \right) \\ & + \left(\frac{\partial I}{\partial R_k} \cdot \frac{\partial R_k}{\partial T_k} + \frac{\partial I}{\partial R_{k+1}} \cdot \frac{\partial R_{k+1}}{\partial T_k} \right), \quad k = 1, \dots, N-1; \end{aligned} \quad (21)$$

$$\frac{\partial I}{\partial T_N} = \frac{\partial I}{\partial G_N} \cdot \frac{\partial G_N}{\partial T_N} + \frac{\partial I}{\partial R_N} \cdot \frac{\partial R_N}{\partial T_N}. \quad (22)$$

A similar result may be established for the level pressure derivatives (not done here). The aerosol concentration profile derivatives are:

$$\frac{\partial I}{\partial x_0} = \frac{\partial I}{\partial A_1} \cdot \frac{\partial A_1}{\partial x_0}; \quad (23)$$

$$\frac{\partial I}{\partial x_k} = \frac{\partial I}{\partial A_k} \cdot \frac{\partial A_k}{\partial x_k} + \frac{\partial I}{\partial A_{k+1}} \cdot \frac{\partial A_{k+1}}{\partial x_k}, \quad k = 1, \dots, N-1; \quad (24)$$

$$\frac{\partial I}{\partial x_N} = \frac{\partial I}{\partial A_N} \cdot \frac{\partial A_N}{\partial x_N}. \quad (25)$$

2.5. Level Jacobians with fine-layer integration

The formulas in Section 2.1 may be readily generalized if there is fine-layer trapezoidal summation. If there are M fine-layer divisions in layer n , then we may write:

$$G_{j,n} = \frac{1}{2}C \sum_{m=1}^M d_{nm} \left(\frac{v_{n,m} p_{n,m} \sigma_{j,n,m}}{T_{n,m}} + \frac{v_{n,m-1} p_{n,m-1} \sigma_{j,n,m-1}}{T_{n,m-1}} \right); \quad (26)$$

$$R_{j,n} = \frac{1}{2}C \varsigma_j \sum_{m=1}^M d_{nm} \left(\frac{p_{n,m}}{T_{n,m}} + \frac{p_{n,m-1}}{T_{n,m-1}} \right); \quad (27)$$

$$A_{j,n} = \frac{1}{2}\epsilon_j \sum_{m=1}^M d_{nm} (x_{n,m} + x_{n,m-1}); \quad (28)$$

Here, we have defined the following fine-layer quantities

$$h_{n,m} = h_{n-1} - \frac{m}{M}(h_{n-1} - h_n), \quad m = 0, \dots, M; \quad (29)$$

$$T_{n,m} = a_{nm}T_{n-1} + b_{nm}T_n; \quad p_{n,m} = (p_{n-1})^{a_{nm}}(p_n)^{b_{nm}}; \quad (30)$$

$$v_{n,m} = a_{nm}v_{n-1} + b_{nm}v_n; \quad x_{n,m} = a_{nm}x_{n-1} + b_{nm}x_n, \quad (31)$$

where

$$a_{nm} = \frac{h_{n,m} - h_n}{h_{n-1} - h_n}; \quad b_{nm} = 1 - a_{nm}; \quad d_{nm} = h_{n,m-1} - h_{n,m}. \quad (32)$$

First, we derive the trace gas VMR profile derivative from a straightforward differentiation of Eq. (26)

$$\frac{\partial G_n}{\partial v_n} = \frac{1}{2}C \sum_{m=1}^M d_{nm} \left(\frac{b_{n,m} q_{j,n,m}}{T_{n,m}} + \frac{b_{n,m-1} q_{j,n,m-1}}{T_{n,m-1}} \right); \quad (33)$$

$$\frac{\partial G_{j,n}}{\partial v_{n-1}} = \frac{1}{2}C \sum_{m=1}^M d_{nm} \left(\frac{a_{n,m} q_{j,n,m}}{T_{n,m}} + \frac{a_{n,m-1} q_{j,n,m-1}}{T_{n,m-1}} \right). \quad (34)$$

Here, we have set $q_{n,m} = p_{n,m}\sigma_{j,n,m}$. Next, we look at temperature derivatives. The Rayleigh derivative for temperature is obtained from Eq. (27):

$$\frac{\partial R_{j,n}}{\partial T_n} = -\frac{1}{2}C_{\zeta_j} \sum_{m=1}^M d_{nm} \left(\frac{b_{n,m}p_{n,m}}{T_{n,m}^2} + \frac{b_{n,m-1}p_{n,m-1}}{T_{n,m-1}^2} \right); \quad (35)$$

$$\frac{\partial R_{j,n}}{\partial T_{n-1}} = -\frac{1}{2}C_{\zeta_j} \sum_{m=1}^M d_{nm} \left(\frac{a_{n,m}p_{n,m}}{T_{n,m}^2} + \frac{a_{n,m-1}p_{n,m-1}}{T_{n,m-1}^2} \right), \quad (36)$$

while the trace gas T-derivatives are:

$$\frac{\partial G_{j,n}}{\partial T_n} = -\frac{1}{2}C \sum_{m=1}^M d_{nm} \left(\frac{b_{n,m}v_{n,m}q_{j,n,m}}{T_{n,m}^2} + \frac{b_{n,m-1}v_{n,m-1}q_{j,n,m-1}}{T_{n,m-1}^2} \right); \quad (37)$$

$$\frac{\partial G_{j,n}}{\partial T_{n-1}} = -\frac{1}{2}C \sum_{m=1}^M d_{nm} \left(\frac{a_{n,m}v_{n,m}q_{j,n,m}}{T_{n,m}^2} + \frac{a_{n,m-1}v_{n,m-1}q_{j,n,m-1}}{T_{n,m-1}^2} \right). \quad (38)$$

Similar results may be written down for the optical depth derivatives with respect to pressure. In addition, the aerosol concentration derivatives may be extracted easily from Eq. (28).

3. Set-ups for Generating Bulk-property Jacobians

So far, we have discussed the generation of profile Jacobians from LIDORT output. Here, we note that LIDORT also has a capacity for generating bulk-property Jacobians $\frac{\partial I}{\partial \chi}$ with respect to some property χ that characterizes or parameterizes the whole atmosphere. This is a useful feature that is much faster than the computation of a series of profile Jacobians which are then summed to obtain a whole-atmosphere Jacobian. The quantity χ might be the total aerosol optical depth or the total ozone column Ω . The latter is required for total ozone retrieval in the UV (325-335 nm) using a direct-fitting regularized least-squares inverse model [7]. In this case, the ozone optical depth profile is regarded as a linear function of Ω when using a column-classified ozone profile climatology, and it is then straightforward to set up the necessary linearized optical inputs required for LIDORT to generate the Jacobian with respect to Ω . In this section we examine Jacobians with respect to temperature shifting, surface-pressure, VMR-scaling setups, and parameterized aerosol loading.

3.1. *T-shift, surface-pressure, VMR-scaling setups*

A temperature shift parameter S is a useful ancillary element to retrieve in situations where there is significant temperature-dependence, but insufficient information content available to retrieve a temperature profile. The direct-fitting total ozone algorithm [7] includes retrieval of this parameter, since the ozone cross-sections in the UV have marked temperature dependence as noted above in section (Rob ADDREF). The temperature shift may be defined through:

$$T_n = \theta_n + S\varphi_n, \quad n = 0, \dots, N \quad (39)$$

where θ_n is the unshifted profile, and φ_n the T-shift shape function. A common setting for the latter is $\varphi_n = 1, \forall n$ (uniform temperature shift).

Since we already have temperature profile derivatives of trace gas absorption optical depths (Eq. 11), the corresponding T-shift derivatives are

$$\frac{\partial G_{j,n}}{\partial S} = \frac{\partial G_{j,n}}{\partial T_n} \varphi_n + \frac{\partial G_{j,n}}{\partial T_{n-1}} \varphi_{n-1}, \quad n = 1, \dots, N \quad (40)$$

A similar result can be written down for the T-shift derivative of the Rayleigh scattering optical depths $R_{j,n}$. From the LIDORT optical property definitions in section 2.3, one can use the chain rule on these equations to write down the required linearized optical property inputs that LIDORT needs to return the T-shift Jacobian.

Derivation of a surface pressure Jacobian is really a corollary of the profile Jacobian transformations in the previous section. As noted in our basic set of assumptions in section 2.1, only those optical properties in the surface layer will depend on the surface pressure P^* . From the basic trace-gas definition in Eq. (1), we find

$$\frac{\partial G_{j,n}}{\partial P^*} = \frac{1}{2} C d_n \frac{v_n \sigma_{j,n}}{T_n}, n = N; \quad \frac{\partial G_{j,n}}{\partial P^*} \equiv 0, n \neq N \quad (41)$$

Similar considerations apply to $\frac{\partial R_{j,n}}{\partial P^*}$. These results then allow us to define the requisite linearized optical property inputs for LIDORT to return this bulk-property Jacobian.

Finally, we look at VMR profile scaling, the idea here being to retrieve a scaling parameter f applied equally to some reference VMR profile $\{v_n^*\}$. The scaled profile is thus $v_n = f v_n^*$, and it follows from sections 2.1 and 2.4 that

$$\frac{\partial G_{j,n}}{\partial f} = \frac{\partial G_{j,n}}{\partial v_n} v_n^* + \frac{\partial G_{j,n}}{\partial v_{n-1}} v_{n-1}^*, \quad n = 1, \dots, N \quad (42)$$

with a similar result again for $\frac{\partial R_{i,n}}{\partial f}$.

3.2. Jacobians for parameterized aerosol loading

The OCO-2 instrument [8] retrieves CO₂ profiles from NIR/SWIR measurements in the O₂ A band and the weak and strong CO₂ bands close to 1.61 μm and 2.04 μm , respectively. Aerosol scattering is dominant, and it is necessary to include ancillary aerosol information in the retrieval. The retrieval will only admit a limited amount of information on the aerosols, and, rather than compute profile Jacobians with respect to the set of aerosol optical thicknesses, it is more reasonable parameterize the aerosol loading in terms of a small number of parameters, and then derive bulk-property Jacobians for these parameters.

It is also more logical to parameterize the aerosol optical properties in terms of the defining microphysical optical parameters (refractive index components) and size distribution parameters, as opposed to developing profile Jacobians with respect to macrophysical aerosol properties such as the layer single scattering albedos. Jacobians for these parameters may be derived through use of a linearized poly-disperse Mie scattering code in conjunction with the linearized RT model. This procedure was investigated for OCO by [9] and is now standard in the OCO-2 algorithm. This combination of codes can also include linearized T-matrix scattering [10].

Here, we confine attention to aerosol loading and consider three parameterizations - a uniform distribution of aerosol characterized by the total amount of aerosol E , an exponentially curved aerosol profile characterized by the total loading E and a relaxation constant k , and a Gaussian profile characterized by the loading E , a peak height z_p and a half width η . It is convenient to express the loading E as the total optical depth of aerosol at one reference wavelength.

- Uniform loading. The uniform case is simplest. If the aerosol is distributed uniformly between levels N_1 and N_2 , then the optical depth profile is

$$A_n = Eq_n = E \frac{(z_{n-1} - z_n)}{(z_{N_1} - z_{N_2})}, \quad n = N_1 + 1, \dots, N_2 \quad (43)$$

and the LIDORT linearized optical inputs with respect to E then follow from Eq (Rob ?) and application of the chain rule to this result.

- Exponential loading. For the exponential case, we can write

$$A(z) = W [e^{-kz_{N_1}} - e^{-kz}], \quad z_{N_1} \geq z \geq z_{N_2} \quad (44)$$

where W is a normalization constant related to total loading E , and $A(z_{N_1}) = 0$. Integration of the profile between limits z_{N_1} and z_{N_2} yields

$$W = \frac{E}{(z_{N_1} - z_{N_2})Y_1 + \frac{1}{k}(Y_1 - Y_2)}; \quad Y_j = e^{-kz_{N_j}} \quad (45)$$

The loading profile is then $A_n = \int_{z_n}^{z_{n-1}} A(z)dz$, which gives

$$A_n = W \left[(z_{n-1} - z_n)Y_1 + \frac{1}{k}(y_{n-1} - y_n) \right]; \quad y_n = e^{-kz_n} \quad (46)$$

Differentiation of Eq.(46) with respect to defining parameters $\{E, k\}$ yields

$$\frac{\partial A_n}{\partial E} = \frac{A_n}{E} \quad (47)$$

$$\frac{\partial A_n}{\partial k} = \frac{A_n}{W} W' + W \left[h_n Y_1' + \frac{1}{k}(y_{n-1}' - y_n') - \frac{1}{k^2}(y_{n-1} - y_n) \right] \quad (48)$$

where the $'$ notation indicates $\partial/\partial k$ and $y_n' = -z_n y_n$ for example. Using the chain rule again, these results allow us to define linearized optical property inputs for LIDORT, and thus to derive aerosol-property Jacobians with respect to E , η and z_p .

- Gaussian loading. For the Gaussian case, we use a GDF (generalized distribution function) profile

$$A(z) = hW \frac{e^{-h(z-z_p)}}{[1 + e^{-h(z-z_p)}]^2}. \quad (49)$$

Here, W is a normalization constant related to total loading E and h is related to the half width η . The advantage here is that the GDF is integrable in simply closed form (no error functions). Indeed, the peak loading is $A(z_p) = \frac{1}{4}W$, the half-width definition implies that

$$h\eta = \ln(3 + \sqrt{8}), \quad (50)$$

and integration of the profile between limits z_{N_1-1} and z_{N_2} yields

$$W = EG; \quad G = \frac{(1 + Y_1)(1 + Y_2)}{(Y_2 - Y_1)}, \quad (51)$$

where $Y_j = \exp[-h(z_{N_j} - z_p)]$ for $j = 1, 2$. It follows that the layer loading profile is

$$A_n = \int_{z_n}^{z_{n-1}} A(z) dz = WP_n; \quad P_n = \frac{(y_n - y_{n-1})}{(1 + y_{n-1})(1 + y_n)}, \quad (52)$$

where $y_n = \exp[-h(z_n - z_p)]$. Differentiation of this last result with respect to the three defining parameters $\{E, \eta, z_p\}$ yields

$$\frac{\partial A_n}{\partial E} = \frac{A_n}{E} \quad (53)$$

$$\frac{\partial A_n}{\partial \eta} = E \left[G \frac{\partial P_n}{\partial \eta} + P_n \frac{\partial G}{\partial \eta} \right] \quad (54)$$

$$\frac{\partial A_n}{\partial z_p} = E \left[G \frac{\partial P_n}{\partial z_p} + P_n \frac{\partial G}{\partial z_p} \right] \quad (55)$$

Derivatives of G and P_n follow from the definitions in Eqs. (51) and (52), and the derivatives of y_n and Y_j . The latter are

$$\frac{\partial y_n}{\partial \eta} = +y_n(z_n - z_p) \frac{h}{\eta}; \quad \frac{\partial y_n}{\partial z_p} = +y_n h. \quad (56)$$

and similarly for derivatives of Y_j . These results allow us to define linearized optical property inputs for LIDORT, and thus derive aerosol-property Jacobians with respect to E , η and z_p .

4. Concluding Remarks

In this note, we have examined the derivation of a number of atmospheric profile and bulk property Jacobians from the LIDORT family of radiative transfer models, focusing in particular on the generation of profile Jacobians at atmospheric level boundaries, and on Jacobians with respect to whole-atmosphere properties such as temperature shift and aerosol loading parameters. These derivations are important for retrieval algorithms and OSSEs requiring the generation of a wide class of weighting functions from the appropriate RT forward models.

Supplementary software to implement these derivations is available from RT Solutions.

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Appendix A. P-T derivatives of Absorption Cross-sections

For a given molecule, the HITRAN data base [11] provides a number of quantities for each absorption line L corresponding to a given transition. These are the line intensity I_L , the line transition lower energy state E_L , the (unshifted) line transition frequency ν_L^* in wavenumbers, a pressure shift coefficient S_L , the air-broadened transition half width α_L at reference temperature T_0 and reference pressure of one atmosphere, and a power-law temperature scaling factor γ_L for this half width. (We have omitted self-broadening). In HITRAN, the reference temperature $T_0 = 296$ K. The ancillary data comprises a set of partition functions $Q(T)$ specified at every 1 K in the range 180-350 K; values at arbitrary temperatures are obtained through 4-point Lagrangian interpolation (essentially a cubic polynomial).

The cross-section at wave number ν is assumed to be a sum of uncorrelated contributions from adjacent lines, and we treat one species independently (no line mixing). The cross-section formula has the following form [12]:

$$\sigma(\nu) = \sum_{L=1}^{N_{lines}} \Psi_L V_L [x_L(\nu), y_L]. \quad (\text{A.1})$$

where $V_L [x_L(\nu), y_L]$ is the Voigt function with arguments $x_L(\nu)$ and y_L such that

$$x_L(\nu) = \frac{(\nu) - \nu_L}{g_L}; \quad (\text{A.2})$$

$$g_L = C \sqrt{\frac{T}{M}} \nu_L; \quad y_L = \frac{\alpha_L \left(\frac{T_0}{T}\right)^{\gamma_L} p}{g_L}. \quad (\text{A.3})$$

Here, T is the temperature, M the species molecular weight, and C the radiation constant. The shifted line position is $\nu_L = \nu_L^* + S_L p$ in terms of the pressure p (in [atm]) and the pressure shift coefficient S_L .

The line-strength factor Ψ_L in Eq. (A.1) is based on local thermodynamic equilibrium and is given by [12]:

$$\Psi_L = \frac{e^{-\frac{E_L k}{T}} \left(1 - e^{-\frac{\nu_L k}{T}}\right)}{e^{-\frac{E_L k}{T_0}} \left(1 - e^{-\frac{\nu_L k}{T_0}}\right)} \cdot \frac{Q(T_0)}{Q(T)} \cdot \frac{I_L}{g_L}. \quad (\text{A.4})$$

where k is second radiation constant = 1.4388 cm K, and $Q(T)$ the partition function at temperature T .

Pressure and temperature derivatives for Eq. (A.1) are

$$\frac{\partial \sigma(\nu)}{\partial P} = \sum_{L=1}^{N_{lines}} \left(\frac{\partial \Psi_L}{\partial P} V_L [x_L(\nu), y_L] + \Psi_L \frac{\partial V_L [x_L(\nu), y_L]}{\partial P} \right); \quad (\text{A.5})$$

$$\frac{\partial \sigma(\nu)}{\partial T} = \sum_{L=1}^{N_{lines}} \left(\frac{\partial \Psi_L}{\partial T} V_L [x_L(\nu), y_L] + \Psi_L \frac{\partial V_L [x_L(\nu), y_L]}{\partial T} \right). \quad (\text{A.6})$$

Derivatives of the Voigt function are usually given with respect to the arguments $x_L(\nu)$ and y_L . Derivatives with respect to T and P derivatives are then

$$\frac{\partial V_L [x_L(\nu), y_L]}{\partial P} = \frac{\partial V_L [x_L, y_L]}{\partial x_L} \frac{\partial x_L}{\partial P} + \frac{\partial V_L [x_L, y_L]}{\partial y_L} \frac{\partial y_L}{\partial P}; \quad (\text{A.7})$$

$$\frac{\partial V_L [x_L(\nu), y_L]}{\partial T} = \frac{\partial V_L [x_L, y_L]}{\partial x_L} \frac{\partial x_L}{\partial T} + \frac{\partial V_L [x_L, y_L]}{\partial y_L} \frac{\partial y_L}{\partial T}, \quad (\text{A.8})$$

where (from the definitions above):

$$\frac{\partial x_L}{\partial P} = -\frac{S_L}{g_L} \left(1 + x_L C \sqrt{\frac{T}{M}}\right) \quad ; \quad \frac{\partial x_L}{\partial T} = -x_L \frac{C}{2T}; \quad (\text{A.9})$$

$$\frac{\partial y_L}{\partial P} = -\frac{y_L \sigma_L^*}{P \sigma_L} \quad ; \quad \frac{\partial y_L}{\partial T} = -\frac{y_L}{T} \left(\gamma_L + \frac{C}{2}\right) \quad (\text{A.10})$$

There is an extensive literature on the Voigt function and its derivatives; see for example the reviews by ([13], [14]). For $y > 0$, the Voigt function $V(x, y)$ is the real part of the scaled complementary error function (also known as the Faddeyeva function) $K(z) \equiv V(x, y) + iL(x, y) = \exp[-z^2] (1 + \text{Erf}(iz))$ for the complex variable $z = x + iy$. In practice, one uses a numerical procedure to provide these quantities. The recent algorithm by Zaghloul [14] is highly

accurate; both x - and y -derivatives are generated. It is common to use a less accurate but faster parameterization of the Voigt function in terms of rational polynomial or exponential functions. For example, the well known Humlicek function [15] is accurate to better than 10^{-4} for the vast majority of cases. However, there are parts of the complex plane where this approximation is less than stellar [14]. To obtain derivatives of the Humlicek function, it is necessary to perform analytic differentiation of polynomial functions of x and y . In our implementation, we have carried out an explicit differentiation of the Humlicek function and use this numerical routine alongside the Zaghoul software, the latter providing benchmark results.

Returning to Eq. (A.1), derivatives of the line-strength factor Ψ_L may be easily obtained from the definition in terms of energy exponentials and partition functions. Energy exponentials have T-derivatives

$$-\frac{E_L k}{T^2} \exp[-E_L k/T] \quad (\text{A.11})$$

for example, while the partition function T-derivatives $\frac{\partial Q(T)}{\partial T}$ may be obtained through explicit differentiation of the Lagrangian interpolation formula. Note that it is also possible to use a more fundamental definition of the partition function in terms of quantum-state population densities - such a definition would need to incorporate knowledge of quantum statistics. However, the temperature derivative in this case is still relatively simple to generate since the partition functions are just weighted sums of exponential factors with exponents inversely proportional to temperature.

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