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Direct linearization and adjoint approaches to evaluation of atmospheric weighting functions and surface partial derivatives: General principles, synergy and areas of application

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1. Subject of discussion

Observable radiances: functionals of atmospheric parameters and functions of surface parameters:

$$R(\mu) = R[\{X(z)\}, \{X_s\}; \mu]$$

Atmospheric weighting functions (WFs) and surface partial derivatives (PDs):

$$\delta_X R(\mu) = \int K^{(X)}(z,\mu)\delta X(z)dz\,, \quad K^{(X)}(z,\mu) = \frac{\delta R(\mu)}{\delta X(z)}$$

$$\delta_{X_s} R(\mu) = K^{(X_s)}(\mu)\delta X_s\,, \quad K^{(X_s)}(\mu) = \frac{\partial R(\mu)}{\partial X_s}$$

Observable radiances are obtained (no matter, consciously or not) from the solution of the (forward) RT problem:

$LI = S\,, \quad R = (W, I)$ **(e.g.,** $R(\mu) = \int\int W(z,u;\mu)I(z,u)dudz$ **)**

For non-scattering atmospheres this can be done analytically, and all WFs and PDs can be computed analytically using the direct linearization approach.

For scattering atmospheres, in general case, the solution of the forward RT problem can be obtained only numerically, but –

Good news: we need only two numerical solutions: one of the forward RT problem and one of the adjoint RT problem to compute all WFs and PDs we can think of.

In this presentation we discuss applications of both the linearization and adjoint approaches

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2. Radiative, individual radiative and geophysical parameters

The forward RT problem $LI = S$ (thermal spectral region):

$$u\frac{dI}{dz} + \alpha(z)\left(I(z,u) - \frac{1}{2}\alpha(z)\int_{-1}^{1} p(z;u,u')I(z,u')du' \right) = \alpha(z)(1-\omega(z))B(z)$$

$$I(0,u) = 0\,, \quad u > 0\,, \quad I(z_0,u) - 2A\int_{0}^{1} I(z_0,u')du' = \varepsilon B_s\,, \quad u < 0$$

Here is the cause-issue chain:

- Observed radiances are determined by radiative parameters that directly enter the forward RT problem:
  - Total extinction coefficient $\alpha(z)$
  - Total phase function $p(z, \cos\Theta)$
  - Atmospheric Planck function $B(z) \equiv \mathrm{B}[T(z)]$
  - Surface Planck function $B_s \equiv \mathrm{B}(T_s)$
- The (total) atmospheric radiative parameters are determined by radiative parameters of individual components (NB! $B(z)$ vs. $T(z)$ is the only exception):

$$\alpha = \sum_k \alpha_k\,, \quad p = \frac{1}{\alpha}\sum_k \alpha_k p_k$$

- The individual radiative parameters are determined by all the multitude of geophysical parameters

3. Inter-links between groups of parameters

Observable radiances are directly related only to (total) radiative parameters entering the forward RT problem through *radiative* WFs and PDs:

$$\delta_B R = \int \frac{\delta R}{\delta B} \delta B dz , \quad \delta_\alpha R = \int \frac{\delta R}{\delta \alpha} \delta \alpha dz , \quad \delta_p R = \int \int K^{(p)}(z,u) \delta p(z,u) dz du$$

$$\delta_{B_s} R = K^{(B_s)} \delta B_s , \quad \delta_\varepsilon R = K^{(\varepsilon)} \delta \varepsilon$$

Perturbations of total atmospheric radiative parameters are directly related only to the individual radiative parameters of atmospheric constituents:

$$\delta_x \alpha = \delta_x \alpha_k , \quad \delta_x p = \frac{1}{\alpha}(p_k - p)\delta_x \alpha_k + \frac{\alpha_k}{\alpha} \delta_x p_k$$

Finally, the individual radiative parameters are directly related to (usually, individual) geophysical parameters; a few examples:

$$\partial \alpha_a / \partial(\ln n_a) = \alpha_a , \quad \partial \ln \alpha_a / \partial m = \partial \ln Q_a / \partial m , \quad \partial \kappa_m / \partial(\ln f_m) = \kappa_m$$

Bottom line: the RT calculations are necessary only for a few radiative WFs and PDs above; the RT calculations are *not necessary at all* (!) for all the multitude of individual geophysical parameters

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4. Blackbody atmospheres and direct linearization approach

A reminder: the observable radiances are functionals wrt atmospheric parameters and are functions wrt the surface parameters: $R(\mu) = R[\{X(z)\},\{X_s\};\mu]$

Analytic implementation of $R[\{X(z)\},\{X_s\};\mu]$ for blackbody atmospheres:

$$R(\mu) = I(0,-\mu) = t(z_0,\mu)\varepsilon B_s + \int_{z_0}^{0} B(z)dt(z,\mu)$$

$$t(z,\mu) = \exp\left(-\tau(z)/\mu\right)$$

$$\tau(z) = \int_0^z \alpha(z')dz'$$

Representing variations $\delta_B R$ and $\delta_\alpha R$ in the form $\delta_X R = \int K^{(X)}(z)\delta X(z)dz$, after some algebra, one can obtain:

$K^{(B)}(z,\mu) = \frac{1}{\mu}\alpha(z)t(z,\mu)$, $K^{(\alpha)}(z,\mu) = -\frac{1}{\mu}[r(z,\mu) - t(z,\mu)B(z)]$, where $r(z,\mu) = t(z_0,\mu)\varepsilon B_s + \int_{z_0}^{z} B(z)dt(z,\mu)$

Similarly, representing variations $\delta_{B_s} R$ and $\delta_\varepsilon R$ in the form $\delta_{X_s} R = K^{(X_s)}\delta X_s$, we obtain:

$$\frac{\partial R(\mu)}{\partial B_s} = t(z_0,\mu)\varepsilon\,, \quad \frac{\partial R(\mu)}{\partial \varepsilon} = t(z_0,\mu)B_s$$

5. Scattering atmospheres and adjoint approach: A concept

The idea: Observables are driven by three entities: L, S, and W, contained in:

- Forward RT problem $LI = S$
- Procedure defining observables $R = (W, I)$.

An alternative way to obtain observables from L, S, and W **is as follows:**

- Define an operator L adjoint to L demanding that $(I^*, LI) = (L^* I^*, I)$;
- Find the solution I^* of the adjoint RT problem $L^* I^* = W$
- Substitute this solution into the definition $(I^*, LI) = (L^* I^*, I)$:

$$(I^*, S) = (W, I) = R$$

This way leads to linearization of observables wrt any RT parameters:

- Linearize the forward RT problem $\delta(LI) = \delta S \rightarrow \delta LI + L\delta I = \delta S \rightarrow L\delta I = \delta S - \delta LI$;
- Substitute into the definition of L^* in the form $(I^*, L\delta I) = (L^* I^*, \delta I)$:

$$(I^*, \delta S - \delta LI) = (W, \delta I) = \delta R$$

Thus, if we perturb any (atmospheric or surface) parameter X, we have:

$$\delta_X R = (I^*, \delta_X S - \delta_X LI)$$

Representing perturbations $\delta_X R = (I^*, \delta_X S - \delta_X LI)$ in the form $\int K^{(X)} \delta X dz$ we can obtain any WF and/or PD from just two solutions: I and I^*.

Isn't it cool?!

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6. Scattering atmospheres and adjoint approach: Implementation

<u>Planck weighting function:</u>

We have: $\delta_B S = \alpha(z)[1-\omega_0(z)]\delta B(z)$, $\delta_B L \equiv 0$ and $\delta_B R = (I^*, \delta_B S) = \int_0^{z_0}\int_{-1}^{1} I^*(z,u)\alpha(z)[1-\omega_0(z)]\delta B(z)\,du\,dz$

We obtain:

$$K^{(B)}(z,\mu) = \alpha(z)[1-\omega_0(z)]\int_{-1}^{1} I^*(z,u;\mu)\,du$$

<u>Extinction coefficient (EC) weighting function:</u>

We have: $\delta_\alpha S - \delta_\alpha L I = \left([1-\omega_0(z)]B(z) - I(z,u) + \frac{1}{2}\int_{-1}^{1} p(z;u,u')I(z,u')\,du'\right)\delta\alpha(z)$, and, in a similar fashion we obtain:

$$K^{(\alpha)}(z,\mu) = \int_{-1}^{1} du\, I^*(z,u;\mu)\left([1-\omega_0(z)]B(z) - I(z,u) + \frac{1}{2}\int_{-1}^{1} p(z;u,u')I(z,u')\,du'\right)$$

<u>If scattering is negligible</u>, $\omega_0 \equiv 0$, and (see JQSRT-05) $I^*(z,u;\mu) = \frac{1}{\mu}t(z,\mu)\delta(u+\mu)$; then we converge to the blackbody results:

$$K^{(B)}(z,\mu) = \frac{1}{\mu}\alpha(z)t(z,\mu), \quad K^{(\alpha)}(z,\mu) = -\frac{1}{\mu}[r(z,\mu) - t(z,\mu)B(z)]$$

7. Implementation of adjoint approach (continued)

Planck partial derivative:

We have: $\delta_{B_s} S = -\delta(z_0 - z)u\theta(-u)\varepsilon\delta B_s$, $\delta_{B_s} L \equiv 0$ and

$$\delta_{B_s} R = (I^*, \delta_{B_s} S) = \int_0^{z_0}\int_{-1}^{1} I^*(z,u)\delta(z_0 - z)(-u)\theta(-u)\varepsilon\delta B_s du dz$$

We obtain:

$$\frac{\partial R(\mu)}{\partial B_s} = \varepsilon \int_{-1}^{0} I^*(z_0, u; \mu)(-u) du$$

Surface emissivity partial derivative:

We have: $\delta_\alpha S - \delta_\alpha L I = \left(B_s - 2\int_0^1 I(z_0, u) u du \right)\delta\varepsilon$, and, in a similar fashion we obtain:

$$\frac{\partial R(\mu)}{\partial \varepsilon} = \int_{-1}^{0} I^*(z_0, u; \mu)(-u) du \cdot \left(B_s - 2\int_0^1 I(z_0, u) du \right)$$

If scattering is negligible, then we obtain:

$$\frac{\partial R(\mu)}{\partial B_s} = t(z_0, \mu)\varepsilon, \quad \frac{\partial R(\mu)}{\partial \varepsilon} = t(z_0, \mu)\left(B_s - 2\int_0^1 I(z_0, u) u du \right)$$

The difference with blackbody results above is due to downward radiation at the ground, neglected there.

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7. Weighting functions for geophysical parameters: Putting all this together

<u>Temperature weighting function</u>

Propagation of variations:

$$\delta T \rightarrow \begin{cases} \delta B \\ \{\delta\alpha_k\} \rightarrow \begin{cases} \delta\alpha \\ \delta p \end{cases} \end{cases}$$

Resulting general expression:

$$K^{(T)} = K^{(B)} \frac{\partial B}{\partial T} + \sum_k \left[K^{(\alpha)} + \frac{1}{\alpha} \int K^{(p)} (p_k - p) du \right] \frac{\partial \alpha_k}{\partial T}$$

If the terms with $K^{(p)}$ are ignored,

$$K^{(T)} = K^{(B)} \frac{\partial B}{\partial T} + K^{(\alpha)} \frac{\partial}{\partial T} \sum_k \alpha_k$$

If temperature dependence of atmospheric extinction is ignored,

$$K^{(T)} = K^{(B)} \frac{\partial B}{\partial T}$$

and, for the blackbody case

$$K^{(T)} = \frac{1}{\mu} \alpha t \frac{\partial B}{\partial T} = \left(-\frac{\partial t}{\partial z} \right) \frac{\partial B}{\partial T}$$

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8. Putting all this together (continued)

<u>Weighting functions for other macrophysical atmospheric parameters</u>

Propagation of variations:

$$\delta X \to \delta\alpha_k \to \begin{cases} \delta\alpha \\ \delta p \end{cases}$$

Resulting general expression:

$$K^{(X)} = \left[K^{(\alpha)} + \frac{1}{\alpha} \int K^{(p)} (p_k - p) du \right] \frac{\partial \alpha_k}{\partial X}$$

If the terms with $K^{(p)}$ are ignored,

$$K^{(X)} = K^{(\alpha)} \frac{\partial \alpha_k}{\partial X}$$

Applications:

- VMR of a minor gaseous constituent: $K^{(\ln f_m)} = K^{(\alpha)} \dfrac{\partial \alpha_m}{\partial \ln f_m} = \alpha_m K^{(\alpha)}$
- Number density of aerosol particles: $K^{(\ln n_a)} = K^{(\alpha)} \dfrac{\partial \alpha_a}{\partial \ln n_a} = \alpha_a K^{(\alpha)}$

9. Putting all this together (continued)

Weighting functions for microphysical atmospheric parameters

Propagation of variations:

$$\delta x \to \begin{cases} \delta\alpha_k \to \begin{cases} \delta\alpha \\ \delta p \end{cases} \\ \delta p_k \to \delta p \end{cases}$$

Resulting general expression:

$$K^{(x)} = \left[K^{(\alpha)} + \frac{1}{\alpha} \int K^{(p)} (p_k - p) du \right] \frac{\partial \alpha_k}{\partial x} + \frac{\alpha_k}{\alpha} \int K^{(p)} \frac{\partial p_k}{\partial x} du$$

If the unperturbed state is represented by a blackbody atmosphere, then $p_k \equiv 0, \quad p \equiv 0,$ and

$$K^{(x)} = K^{(\alpha)} \frac{\partial \alpha_k}{\partial x} + \frac{\alpha_k}{\alpha} \int K^{(p)} \frac{\partial p_k}{\partial x} du$$

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10. Synergy of the direct linearization and adjoint approaches

Synergy:

- Etymology: from Greek *synergos* – working together
- Meaning: a mutually advantageous conjunction of distinct elements
  (Merriam Webster Dictionary)

1st level of synergy:

- Both approaches confine RT computations of WFs and PDs to, at most, five *radiative* WFs and PDs: $\delta R / \delta B$, $\delta R / \delta \alpha$, $\delta R / \delta p$, $\partial R / \partial B_s$, $\partial R / \partial \varepsilon$
- Relations between the cumulative and individual RT parameters of the atmosphere are unified and do not depend on individual geophysical parameters
- Only relations between individual RT parameters and geophysical parameters are indeed *individual*

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8. Synergy of direct linearization and adjoint approaches (ctd.)

2nd level of synergy: Is based on the use of the source functions of the forward RT problem:

$$B(z,u)=[1-\omega_0(z)]B(z)+\frac{1}{2}\int_{-1}^{1}p(z,u;u')I(z,u')du'$$

$$B_s(u)=\varepsilon B_s+(1-\varepsilon)\cdot 2\int_{0}^{1}I(z,u')u'du'$$

(see details in JQSRT-05). Observable radiances become looking like blackbody radiances. Compare:

$$R(\mu)=t(z_0,\mu)B_s(-\mu)+\int_{z_0}^{0}B(z,-\mu)dt(z,\mu),\ \text{and}\ R(\mu)=t(z_0,\mu)\varepsilon B_s+\int_{z_0}^{0}B(z)dt(z,\mu)$$

Atmospheric weighting functions and surface partial derivatives look like combinations of blackbody and adjoint expressions. E.g.,

$$K^{(B)}(z,\mu)=\alpha(z)[1-\omega_0(z)]\left(\int_{-1}^{1}I^*(z,u;\mu)du+\frac{1}{\mu}t(z,u)\right),\ \text{and}\ K^{(B)}(z,\mu)=\alpha(z)\frac{1}{\mu}t(z,u)$$

or

$$K^{(B_s)}(\mu)=\varepsilon\left(\int_{-1}^{0}I^*(z_0,u;\mu)(-u)du+t(z_0,u)\right),\ \text{and}\ K^{(B_s)}(\mu)=\varepsilon\cdot t(z_0,u)$$

Synergy of two approaches is useful, to say the least

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9. Conclusion

- Both linearization and adjoint approach confine RT computations to five, at most, WFs and PDs; the rest is manipulation of individual radiative and geophysical parameters

- The links between cumulative and individual RT parameters are independent on individual RT parameters and can be unified

- Only links between individual RT and geophysical parameters are specific and are unique for retrievals of specific geophysical parameters

- Last, but by no means least:
  - The science that starts after the (linearized) inverse problem $\mathbf{Kx=y}$ is formulated, is well developed;
  - The science that ends after the problem $\mathbf{Kx=y}$ is formulated, needs more development;
  - This science promises development of fast *and* more accurate algorithms; this science certainly deserves more development

Backup Charts

Comparison with the approach based on the linearized RT equation

Linearization (perturbation) of the forward RT problem $LI = S$:

$$\delta(LI) = \delta S \rightarrow \delta L I + L \delta I = \delta S \rightarrow L \delta I = \delta S - \delta L I$$

Corresponding perturbation of the observables $R = (W, I)$:

$$\delta R = (W, \delta I)$$

Arbitrary atmospheric WFs and surface PDs:

$$\frac{\delta R}{\delta X} = \left(W, \frac{\delta I}{\delta X}\right), \quad \frac{\partial R}{\partial X_s} = \left(W, \frac{\partial I}{\partial X_s}\right)$$

Correspondingly, we need the solutions of linearized RT problems:

$$L\frac{\delta I}{\delta X} = \frac{\delta S}{\delta X} - \frac{\delta L}{\delta X} I, \quad L\frac{\partial I}{\partial X_s} = \frac{\partial S}{\partial X_s} - \frac{\partial L}{\partial X_s} I$$

We need *five* solutions for five radiative parameters. Using adjoint approach, we need only *two* solutions. Your opinion solicited.