Mixing Ratio First and Second Derivatives in Linear and Logarithmic Basis

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1 Mixing Ratio First Derivatives

For k and $\tilde{k}$ state vector components (mixing ratio species), $x = f_q^k$ and $y = f_{\tilde{q}}^{\tilde{k}}$ above. Here, q and $\tilde{q}$ are breakpoints where f^k and $f^{\tilde{k}}$ are known. Note that since $\dfrac{\partial \triangle B_i}{\partial f_q^k} = 0$ for all k and q, we have

$$\frac{\partial I(\mathbf{x})}{\partial f_q^k} = -\sum_{i=1}^{2N} \triangle B_i \mathcal{W}_{i,q}^k \mathcal{T}_i, \tag{1}$$

where

$$\mathcal{W}_{1,q}^k = 0,$$
$$\mathcal{W}_{i,q}^k = \mathcal{W}_{i-1,q}^k + \frac{\partial \triangle \delta_{i \to i-1}}{\partial f_q^k}.$$

Opacity Derivatives

The species incremental opacity integral is

$$\triangle \delta_{i \to i-1}^k = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\, \beta^k\, \frac{ds}{dh}\, \frac{dh}{d\zeta}\, d\zeta.$$

Linear basis: Mixing ratios are given by

$$F^k(\zeta) = \sum_{q=1}^{Q} f_q^k \eta_q^k(\zeta),$$

and

$$\frac{\partial F^k}{\partial f_q^k} = \eta_q^k(\zeta).$$

The opacity derivative with respect to mixing ratio using the *linear* basis is

$$\frac{\partial \triangle \delta_{i \to i-1}^k}{\partial f_q^k} = \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^k(\zeta)\, \beta^k\, \frac{ds}{dh}\, \frac{dh}{d\zeta}\, d\zeta. \tag{2}$$

Logarithmic basis: Mixing ratios are given by

$$F^k(\zeta) = \exp\left[\sum_{q=1}^{Q} \log f_q^k \eta_q^k(\zeta)\right],$$

and

$$\frac{\partial F^k}{\partial f_q^k} = F^k(\zeta)\frac{\eta_q^k(\zeta)}{f_q^k}.$$

The opacity derivative with respect to mixing ratio using the *logarithmic* basis is

$$\frac{\partial \triangle \delta_{i\to i-1}^k}{\partial f_q^k} = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\frac{\eta_q^k(\zeta)}{f_q^k}\,\beta^k\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta. \tag{3}$$

Remark: For both linear and logarithmic basis, we have

$$\frac{\partial F^k}{\partial f_q^{\tilde{k}}} = 0, \;\; \text{for } k \neq \tilde{k},$$

and hence

$$\frac{\partial \triangle \delta_{i\to i-1}^k}{\partial f_q^{\tilde{k}}} = 0, \;\; \text{for } k \neq \tilde{k},$$

where k and $\tilde{k}$ are molecules.

Note that $\dfrac{\partial \triangle \delta_{i\to i-1}}{\partial f_q^k} = \dfrac{\partial}{\partial f_q^k}\Big(\sum_k \triangle \delta_{i\to i-1}^k\Big) = \dfrac{\partial \triangle \delta_{i\to i-1}^k}{\partial f_q^k}.$

2 Mixing Ratio Second Derivatives

Note that since $\dfrac{\partial \triangle B_i}{\partial f_q^k} = 0$ and $\dfrac{\partial^2 \triangle B_i}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = 0$, we have

$$\frac{\partial^2 I(\mathbf{x})}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = \sum_{i=1}^{2N} \triangle B_i \left(\mathcal{W}_{i,q}^k \mathcal{W}_{i,\tilde{q}}^{\tilde{k}} - \partial \mathcal{W}_{i,q,\tilde{q}}^{k,\tilde{k}} \right) \mathcal{T}_i, \tag{4}$$

where

$$\begin{aligned}
\mathcal{W}_{1,q}^k &= 0, \quad \partial \mathcal{W}_{1,q,\tilde{q}}^k = 0, \\
\mathcal{W}_{i,q}^k &= \mathcal{W}_{i-1,q}^k + \frac{\partial \triangle \delta_{i\to i-1}}{\partial f_q^k}, \\
\partial \mathcal{W}_{i,q,\tilde{q}}^{k,\tilde{k}} &= \partial \mathcal{W}_{i-1,q,\tilde{q}}^{k,\tilde{k}} + \frac{\partial^2 \triangle \delta_{i\to i-1}}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}}.
\end{aligned}$$

Opacity Second Derivatives

Linear basis: The opacity second derivative with respect to mixing ratios using the *linear* basis, for molecules k and $\tilde{k}$, is identically 0:

$$\frac{\partial^2 \triangle \delta_{i\to i-1}^k}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} = \int_{\zeta_i}^{\zeta_{i-1}} \frac{\partial \eta_q^k(\zeta)}{\partial f_{\tilde{q}}^{\tilde{k}}}\,\beta^k\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta = 0, \tag{5}$$

for all k, $\tilde{k}$ and q, $\tilde{q}$. Thus,

$$\partial \mathcal{W}_{i,q,\tilde{q}}^{k,\tilde{k}} = 0,$$

and

$$\frac{\partial^2 I(\mathbf{x})}{\partial f_q^k \partial f_{\tilde{q}}^k} = \sum_{i=1}^{2N} \triangle B_i \mathcal{W}_{i,q}^k \mathcal{W}_{i,\tilde{q}}^{\tilde{k}} \mathcal{T}_i. \tag{6}$$

2

Logarithmic basis: The opacity second derivative with respect to mixing ratios using the *logarithmic* basis, for molecules k and $\tilde{k}$, is:

$$\frac{\partial^2 \triangle \delta^k_{i \to i-1}}{\partial f^k_q \partial f^k_q} \quad = \quad \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\, \beta^k\, \frac{\eta^k_q(\zeta)}{(f^k_q)^2} \Big[\eta^k_q(\zeta) - 1 \Big] \frac{ds}{dh} \frac{dh}{d\zeta}\, d\zeta, \tag{7}$$

$$\frac{\partial^2 \triangle \delta^k_{i \to i-1}}{\partial f^k_q \partial f^k_{\tilde{q}}} \quad = \quad \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\, \beta^k\, \frac{\eta^k_q(\zeta)\eta^k_{\tilde{q}}(\zeta)}{f^k_q f^k_{\tilde{q}}} \frac{ds}{dh} \frac{dh}{d\zeta}\, d\zeta, \qquad q \neq \tilde{q}, \tag{8}$$

which can also be written as

$$\frac{\partial^2 \triangle \delta^k_{i \to i-1}}{\partial f^k_q \partial f^k_{\tilde{q}}} \quad = \quad \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\, \beta^k\, \frac{\eta^k_q(\zeta)}{f^k_q f^k_{\tilde{q}}} \Big[\eta^k_{\tilde{q}}(\zeta) - d_{q\tilde{q}} \Big] \frac{ds}{dh} \frac{dh}{d\zeta}\, d\zeta, \tag{9}$$

$$\text{where} \quad d_{q\tilde{q}} \quad = \quad \begin{cases} 1, & q = \tilde{q}, \\ 0, & q \neq \tilde{q} \end{cases} \quad \text{is the Dirac delta function.}$$

Note that

$$\frac{\partial^2 \triangle \delta^k_{i \to i-1}}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} = 0 \quad \text{for} \quad k \neq \tilde{k}. \tag{10}$$

The mixing ratio second derivatives using the logarithmic basis are evaluated as in (4):

$$\frac{\partial^2 I(\mathbf{x})}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} \quad = \quad \sum_{i=1}^{2N} \triangle B_i \left(\mathcal{W}^k_{i,q}\, \mathcal{W}^{\tilde{k}}_{i,\tilde{q}} - \partial\mathcal{W}^{k,\tilde{k}}_{i,q,\tilde{q}} \right) \mathcal{T}_i.$$

Remark: If k is in **linear basis** and $\tilde{k}$ is in **logarithmic basis**, the mixing ratio second derivatives are evaluated as

$$\frac{\partial^2 I(\mathbf{x})}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} \quad = \quad \sum_{i=1}^{2N} \triangle B_i \mathcal{W}^k_{i,q}\, \mathcal{W}^{\tilde{k}}_{i,\tilde{q}}\, \mathcal{T}_i.$$

The first order opacity derivatives for k and $\tilde{k}$ are given by equations (2) and (3), respectively. See equation (10).

Remark: Here, we assume linear basis. Since

$$\frac{\partial I}{\partial f^k_q} \quad = \quad \sum_{i=1}^{2N} \triangle B_i \frac{\partial \mathcal{T}_i}{\partial f^k_q} \quad \text{and} \quad \frac{\partial^2 I}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} \quad = \quad \sum_{i=1}^{2N} \triangle B_i \frac{\partial^2 \mathcal{T}_i}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}},$$

radiative transfer mixing ratio first and second derivatives can be computed after evaluating

derivatives of $\mathcal{T}_i$:

$$
\begin{aligned}
\frac{\partial \mathcal{T}_i}{\partial f_q^k} &= \frac{\partial}{\partial f_q^k}\left[\exp\left(-\sum_{j=2}^{i}\triangle\delta_{j\to j-1}\right)\right] \\
&= \frac{\partial}{\partial f_q^k}\left[\exp\left(-\sum_{j=2}^{i}\sum_{k}\int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta\right)\right] \\
&= -\mathcal{T}_i\sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}}\eta_q^k\beta^k\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta, \\
\frac{\partial^2 \mathcal{T}_i}{\partial f_q^k \partial f_{\tilde{q}}^{\tilde{k}}} &= \mathcal{T}_i\left(\sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}}\eta_q^k\beta^k\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta\right)\left(\sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}}\eta_{\tilde{q}}^{\tilde{k}}\beta^{\tilde{k}}\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta\right),
\end{aligned}
$$

which are consistent with results obtained in (1) and (6).

Examples

O_3 molecules

The opacity derivative with respect to O_3 mixing ratio using the linear basis is

$$
\frac{\partial \triangle\delta_{i\to i-1}^{O_3}}{\partial f_q^{O_3}} = \int_{\zeta_i}^{\zeta_{i-1}}\eta_q^{O_3}(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta.
$$

The **derivative of the radiative transfer** is

$$
\frac{\partial I(\mathbf{x})}{\partial f_q^{O_3}} = -\sum_{i=1}^{2N}\triangle B_i\mathcal{W}_{i,q}^{O_3}\mathcal{T}_i,
$$

where

$$
\begin{aligned}
\mathcal{W}_{1,q}^{O_3} &= 0, \\
\mathcal{W}_{i,q}^{O_3} &= \mathcal{W}_{i-1,q}^{O_3} + \frac{\partial \triangle\delta_{i\to i-1}}{\partial f_q^{O_3}}.
\end{aligned}
$$

For all i and q, calculate

$$
\frac{\partial \triangle\delta_{i\to i-1}^{O_3}}{\partial f_q^{O_3}} = \int_{\zeta_i}^{\zeta_{i-1}}\eta_q^{O_3}(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta.
$$

Given $W_{i,q}^{O_3}$, compute

$$
\frac{\partial I_l}{\partial f_q^{O_3}} = -\sum_{i=1}^{2N}\triangle B_i\mathcal{W}_{i,q}^{O_3}\mathcal{T}_i,
$$

where l is the level number (path) above the Earth surface. For a higher level l, there are more i's with $\mathcal{T}_i = 0$.

O_3 and N_2 molecules

The opacity derivatives with respect to O_3 and N_2 mixing ratios using the linear basis are

$$
\begin{aligned}
\frac{\partial \triangle\delta_{i\to i-1}^{O_3}}{\partial f_q^{O_3}} &= \int_{\zeta_i}^{\zeta_{i-1}}\eta_q^{O_3}(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta, \\
\frac{\partial \triangle\delta_{i\to i-1}^{N_2}}{\partial f_q^{N_2}} &= \int_{\zeta_i}^{\zeta_{i-1}}\eta_q^{N_2}(\zeta)\,\beta^{N_2}\,\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta.
\end{aligned}
$$

4

Since **incremental opacity** is given by

$$\triangle\delta_{i\to i-1} = \triangle\delta^{O_3}_{i\to i-1} + \triangle\delta^{N_2}_{i\to i-1},$$

we have

$$\frac{\partial\triangle\delta_{i\to i-1}}{\partial f_q^{O_3}} = \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^{O_3}(\zeta)\beta^{O_3}\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta,$$

$$\frac{\partial\triangle\delta_{i\to i-1}}{\partial f_q^{N_2}} = \int_{\zeta_i}^{\zeta_{i-1}} \eta_q^{N_2}(\zeta)\beta^{N_2}\frac{ds}{dh}\frac{dh}{d\zeta}\,d\zeta.$$

The derivative of the radiative transfer is

$$\frac{\partial I(\mathbf{x})}{\partial f_q^k} = -\sum_{i=1}^{2N}\triangle B_i \mathcal{W}_{i,q}^k \mathcal{T}_i,$$

where

$$\mathcal{W}_{1,q}^k = 0,$$

$$\mathcal{W}_{i,q}^k = \mathcal{W}_{i-1,q}^k + \frac{\partial\triangle\delta_{i\to i-1}}{\partial f_q^k},$$

where k is either O_3 or N_2.