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

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

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

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

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

$$\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f^k_q} = \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\frac{\eta^k_q(\zeta)}{f^k_q}\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

Remark: For both linear and logarithmic basis, we have

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

and

$$\frac{\partial \triangle\delta^k_{i\to i-1}}{\partial f^{\tilde{k}}_q} = 0,\;\; \text{for } k \neq \tilde{k},$$

where k and $\tilde{k}$ are molecules.
Note that $\dfrac{\partial \triangle\delta_{i\to i-1}}{\partial f^k_q} = \dfrac{\partial}{\partial f^k_q}\Big(\sum_k \triangle\delta^k_{i\to i-1}\Big) = \dfrac{\partial \triangle\delta^k_{i\to i-1}}{\partial f^k_q}$.

2 Mixing Ratio Second Derivatives

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

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

where

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

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:

$$\begin{aligned}
\frac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} &= \int_{\zeta_i}^{\zeta_{i-1}} \frac{\partial \eta^k_q(\zeta)}{\partial f^{\tilde{k}}_{\tilde{q}}}\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\\
&= 0,
\end{aligned}$$

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

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

and

$$\frac{\partial^2 I(\mathbf{x})}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} \;=\; \sum_{i=1}^{2N} \triangle B_i \mathcal{W}^k_{i,q}\mathcal{W}^{\tilde{k}}_{i,\tilde{q}}\,\mathcal{T}_i. \tag{3}$$

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

$$
\begin{aligned}
\frac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f^k_q \partial f^k_q} &= \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{\eta^k_q(\zeta)}{(f^k_q)^2}\Big[\eta^k_q(\zeta)-1\Big]\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,\\
\frac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f^k_q \partial f^k_{\tilde{q}}} &= \int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{\eta^k_q(\zeta)\eta^k_{\tilde{q}}(\zeta)}{f^k_q f^k_{\tilde{q}}}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta, \qquad q \neq \tilde{q},
\end{aligned}
$$

which can also be written as

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

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

Note that $\dfrac{\partial^2 \triangle\delta^k_{i\to i-1}}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} = 0$ for $k \neq \tilde{k}$.

The mixing ratio second derivatives using the logarithmic basis are evaluated as in (2):

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

Remark: Assuming linear basis, since

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

radiative transfer mixing ratio first and second derivatives can be computed after evaluating derivatives of $\mathcal{T}_i$:

$$
\begin{aligned}
\frac{\partial \mathcal{T}_i}{\partial f^k_q} &= \frac{\partial}{\partial f^k_q}\Big[\exp\Big(-\sum_{j=2}^{i} \triangle\delta_{j\to j-1}\Big)\Big]\\
&= \frac{\partial}{\partial f^k_q}\Big[\exp\Big(-\sum_{j=2}^{i}\sum_{k}\int_{\zeta_i}^{\zeta_{i-1}} F^k(\zeta)\,\beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\Big)\Big]\\
&= -\mathcal{T}_i \sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}} \eta^k_q \beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta,\\
\frac{\partial^2 \mathcal{T}_i}{\partial f^k_q \partial f^{\tilde{k}}_{\tilde{q}}} &= \mathcal{T}_i \Big(\sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}} \eta^k_q \beta^k\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\Big)\Big(\sum_{j=2}^{i}\int_{\zeta_i}^{\zeta_{i-1}} \eta^{\tilde{k}}_{\tilde{q}} \beta^{\tilde{k}}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta\Big),
\end{aligned}
$$

which are consistent with results obtained in (1) and (3).

Examples

O_3 molecules

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

$$\frac{\partial \triangle \delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} = \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

The **derivative of the radiative transfer** is

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

where

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

For all i and q, calculate

$$\frac{\partial \triangle \delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} = \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.$$

Given $W^{O_3}_{i,q}$, compute

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

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

$$\begin{aligned}
\frac{\partial \triangle \delta^{O_3}_{i\to i-1}}{\partial f^{O_3}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{O_3}_q(\zeta)\,\beta^{O_3}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta, \\
\frac{\partial \triangle \delta^{N_2}_{i\to i-1}}{\partial f^{N_2}_q} &= \int_{\zeta_i}^{\zeta_{i-1}} \eta^{N_2}_q(\zeta)\,\beta^{N_2}\,\frac{ds}{dh}\,\frac{dh}{d\zeta}\,d\zeta.
\end{aligned}$$

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

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

The derivative of the radiative transfer is

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

where

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

where k is either O_3 or N_2.