Derivation of Jacobian matrix

Given n+1 components in a melt with their concentrations w_1, $\dots w_n$ and w_{n+1}, let's choose the n+1th component as the dependent component and derive their derivatives with respect to eigenvectors and eigenvalues as well as interface position.

Define w as follows:

$$\boldsymbol{w} = (w_1, w_2, \dots, w_n)^T \tag{1}$$

where

$$w_{n+1} = 1 - \sum_{i=1}^{n} w_i \tag{2}$$

For diffusion couple:

$$\boldsymbol{w} = \frac{\boldsymbol{w_2}+\boldsymbol{w_1}}{2} + P \times E \times P^{-1} \times \frac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} \tag{3}$$

where

$$E = \begin{pmatrix} \operatorname{erf}\left(\frac{x-x_0}{\sqrt{4e^{\beta_1}t}}\right) & & \\ & \ddots & \\ & & \operatorname{erf}\left(\frac{x-x_0}{\sqrt{4e^{\beta_n}t}}\right) \end{pmatrix}$$

$$= \begin{pmatrix} \operatorname{erf}\left(\frac{x-x_0}{\sqrt{4t}}e^{-\frac{\beta_1}{2}}\right) & & \\ & \ddots & \\ & & \operatorname{erf}\left(\frac{x-x_0}{\sqrt{4t}}e^{-\frac{\beta_n}{2}}\right) \end{pmatrix} \tag{4}$$

Define $\boldsymbol{\beta}$ as follows:

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} \tag{5}$$

Define $\boldsymbol{Y}$ as follows:

$$\boldsymbol{Y} = \begin{pmatrix} \frac{x-x_0}{\sqrt{4t}}e^{-\frac{\beta_1}{2}} \\ \vdots \\ \frac{x-x_0}{\sqrt{4t}}e^{-\frac{\beta_n}{2}} \end{pmatrix} = \frac{x-x_0}{\sqrt{4t}}e^{-\frac{\boldsymbol{\beta}}{2}} \tag{6}$$

Then

$$E = diag\begin{pmatrix} \text{erf}\left(\frac{x-x_0}{\sqrt{4t}} e^{-\frac{\beta_1}{2}}\right) \\ \vdots \\ \text{erf}\left(\frac{x-x_0}{\sqrt{4t}} e^{-\frac{\beta_n}{2}}\right) \end{pmatrix} = diag\big(\text{erf}\,(\boldsymbol{Y})\big) \tag{7}$$

Take the total differential of $\boldsymbol{w}$:

$$\begin{aligned} \mathbf{d}\,\boldsymbol{w} = \mathbf{d}\,P \times E \times P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} + P \times \mathbf{d}\,E \times P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} \\ + P \times E \times \mathbf{d}\,P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} \end{aligned} \tag{8}$$

According to Eq. (7),

$$\begin{aligned} \mathbf{d}\,E &= \mathbf{d}\,diag(\text{erf}(\boldsymbol{Y})) \\ &= diag(\mathbf{d}\,\text{erf}(\boldsymbol{Y})) \\ &= diag\left(\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \mathbf{d}\,\boldsymbol{Y}\right) \\ &= diag\left(\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \mathbf{d}\left(\frac{x-x_0}{\sqrt{4t}} e^{-\frac{\boldsymbol{\beta}}{2}}\right)\right) \\ &= diag\left(\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \left(\frac{x-x_0}{\sqrt{4t}} * \left(-\frac{1}{2}\right) * e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta} - \frac{1}{\sqrt{4t}}\, e^{-\frac{\boldsymbol{\beta}}{2}} \mathbf{d} x_0\right)\right) \\ &= -\frac{x-x_0}{\sqrt{4\pi t}} diag\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta}\right) - \frac{1}{\sqrt{\pi t}} diag\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \mathbf{d}\,x_0 \\ &= -\frac{x-x_0}{\sqrt{4\pi t}} diag\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \odot \mathbf{d}\,(diag\,\boldsymbol{\beta}) - \frac{1}{\sqrt{\pi t}} diag\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \mathbf{d}\,x_0 \\ &= -\tfrac{x-x_0}{\sqrt{4\pi t}} dE \odot \mathbf{d}\,(diag\,\boldsymbol{\beta}) - \tfrac{1}{\sqrt{\pi t}} dE\,\mathbf{d}\,x_0 \end{aligned} \tag{9}$$

where

$$dE = diag\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \tag{10}$$

Therefore,

$$\begin{aligned} P \times \mathbf{d}\,E \times P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} = -\tfrac{x-x_0}{\sqrt{4\pi t}} P \times \big(dE \odot \mathbf{d}\,(diag\,\boldsymbol{\beta})\big) \times P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} \\ - \tfrac{1}{\sqrt{\pi t}} P \times dE \times P^{-1} \times \tfrac{\boldsymbol{w_2}-\boldsymbol{w_1}}{2} \mathbf{d}\,x_0 \end{aligned} \tag{11}$$

To calculate $\mathbf{d}\,P^{-1}$,

$$\mathbf{d}\, P^{-1} = -P^{-1} \times \mathbf{d}\, P \times P^{-1} \tag{12}$$

Plug Eq. (11) and Eq. (12) into Eq. (8)

$$\begin{aligned}
\mathbf{d}\, \boldsymbol{w} &= \mathbf{d}\, P \times E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2} \\
&- \frac{x - x_0}{\sqrt{4\pi t}} P \times \left(dE \odot \mathbf{d}\, (diag\, \boldsymbol{\beta})\right) \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2} \\
&- \frac{1}{\sqrt{\pi t}} P \times dE \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2} \mathbf{d}\, x_0 \\
&- P \times E \times P^{-1} \times \mathbf{d}\, P \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}
\end{aligned} \tag{13}$$

Take the vectorization of each term of Eq. (13),

$$\begin{aligned}
& vec\left(\mathbf{d}\, P \times E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \\
&= \left(\left(E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{\mathrm{T}} \otimes I_n\right) \times vec(\mathbf{d}\, P)
\end{aligned} \tag{14}$$

$$\begin{aligned}
& vec\left(-\frac{x - x_0}{\sqrt{4\pi t}} P \times \left(dE \odot \mathbf{d}\, (diag\, \boldsymbol{\beta})\right) \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \\
&= -\frac{x - x_0}{\sqrt{4\pi t}} \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes P\right) \times vec\left(\left(dE \odot \mathbf{d}\, (diag\, \boldsymbol{\beta})\right)\right) \\
&= -\frac{x - x_0}{\sqrt{4\pi t}} \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes P\right) \times diag\left(vec(dE)\right) \times vec\left(\mathbf{d}\, (diag\, \boldsymbol{\beta})\right)
\end{aligned} \tag{15}$$

and

$$\begin{aligned}
& vec\left(-P \times E \times P^{-1} \times \mathbf{d}\, P \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \\
&= -\left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes (P \times E \times P^{-1})\right) \times vec(\mathbf{d}\, P)
\end{aligned} \tag{16}$$

Therefore, the vectorization of $\mathbf{d}\, \boldsymbol{w}$ is

$$vec(\mathbf{d}\, \boldsymbol{w})$$

$$= \left\{\left(\left(E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{\mathrm{T}} \otimes I_n\right) - \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes (\, P \times E \times P^{-1}\,)\right)\right\} \times vec(\mathrm{d}P)$$

$$- \frac{x - x_0}{\sqrt{4\pi t}} \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes P\right) \times diag\big(vec(dE)\big) \times vec\big(\mathbf{d}\ (diag\ \boldsymbol{\beta})\big)$$

$$- \frac{1}{\sqrt{\pi t}} P \times dE \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2} \mathbf{d}\ x_0 \tag{17}$$

Therefore,

$$w_{x_0} = -\frac{1}{\sqrt{\pi t}} \left(P \times dE \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \tag{18}$$

$$w_P = \frac{\partial w}{\partial P} = \left\{\left(\left(E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{\mathrm{T}} \otimes I_n\right) - \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes (\, P \times E \times P^{-1}\,)\right)\right\}^{T}$$

$$= \left(\left(E \times P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \quad \otimes I_n\right) - \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \quad \otimes (P \times E \times P^{-1})^{T}\right) \tag{19}$$

and

$$w_{diag\ \boldsymbol{\beta}} = \frac{\partial w}{\partial diag\ \boldsymbol{\beta}} = -\frac{x - x_0}{\sqrt{4\pi t}} \left\{\left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right)^{T} \otimes P\right) \times diag\big(vec(dE)\big)\right\}^{T}$$

$$= -\frac{x - x_0}{\sqrt{4\pi t}} diag\big(vec(dE)\big) \times \left(\left(P^{-1} \times \frac{\boldsymbol{w_2} - \boldsymbol{w_1}}{2}\right) \quad \otimes P^{T}\right) \tag{20}$$

To get $\frac{\partial w_{n+1}}{\partial x_0}$, $\frac{\partial w_{n+1}}{\partial P}$, and $\frac{\partial w_{n+1}}{\partial diag\ \boldsymbol{\beta}}$:

$$\frac{\partial w_{n+1}}{\partial x_0} = -\sum_i^n w_{x_0}\,(:, i) \tag{21}$$

$$\frac{\partial w_{n+1}}{\partial P} = -\sum_i^n w_P\,(:, i) \tag{22}$$

$$\frac{\partial w_{n+1}}{\partial diag\ \boldsymbol{\beta}} = -\sum_i^n w_{diag\ \boldsymbol{\beta}}\,(:, i) \tag{23}$$

Since $\boldsymbol{r} = {}^{(\boldsymbol{w_0} - \boldsymbol{w}\quad).}/_{\boldsymbol{\sigma}}$, we have

$$r_{x_0} = {}^{-w_{x_0}.}/_{\sigma} \tag{24}$$

$$r_P = {}^{-w_P\,.}/_{\sigma} \tag{25}$$

$$r_{diag\ \boldsymbol{\beta}} = {}^{-w_{diag\ \boldsymbol{\beta}}.}/_{\sigma} \tag{26}$$

To get $\frac{\partial r_{n+1}}{\partial x_0}$, $\frac{\partial r_{n+1}}{\partial P}$ and $\frac{\partial r_{n+1}}{\partial diag\ \boldsymbol{\beta}}$:

$$\frac{\partial r_{n+1}}{\partial x_0} = \left(\sum_i^n w_{x_0}\,(:,i)\right)\Big/\sigma_{n+1} \tag{27}$$

$$\frac{\partial r_{n+1}}{\partial P} = \left(\sum_i^n w_P\,(:,i)\right)\Big/\sigma_{n+1} \tag{28}$$

$$\frac{\partial r_{n+1}}{\partial diag\,\boldsymbol{\beta}} = \left(\sum_i^n w_{diag\,\boldsymbol{\beta}}\,(:,i)\right)\Big/\sigma_{n+1} \tag{29}$$

For mineral dissolution:

$$w = w_{initial} + P \times E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \tag{30}$$

where

$$E_{ratio} = \begin{pmatrix} \frac{\operatorname{erfc}\left(\frac{x-L}{\sqrt{4e^{\beta_1}t}}\right).}{\operatorname{erfc}\left(\frac{-L}{\sqrt{4e^{\beta_1}t}}\right)} & & \\ & \ddots & \\ & & \frac{\operatorname{erfc}\left(\frac{x-L}{\sqrt{4e^{\beta_n}t}}\right).}{\operatorname{erfc}\left(\frac{-L}{\sqrt{4e^{\beta_n}t}}\right)} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\operatorname{erfc}\left(\frac{x-L}{\sqrt{4t}}e^{-\frac{\beta_1}{2}}\right).}{\operatorname{erfc}\left(\frac{-L}{\sqrt{4t}}e^{-\frac{\beta_1}{2}}\right)} & & \\ & \ddots & \\ & & \frac{\operatorname{erfc}\left(\frac{x-L}{\sqrt{4t}}e^{-\frac{\beta_n}{2}}\right).}{\operatorname{erfc}\left(\frac{-L}{\sqrt{4t}}e^{-\frac{\beta_n}{2}}\right)} \end{pmatrix} \tag{31}$$

Define $\boldsymbol{\beta}$ as follows:

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} \tag{32}$$

Define $\boldsymbol{Y}$ and $\boldsymbol{Y_0}$ as follows:

$$\boldsymbol{Y} = \begin{pmatrix} \frac{x-L}{\sqrt{4t}}e^{-\frac{\beta_1}{2}} \\ \vdots \\ \frac{x-L}{\sqrt{4t}}e^{-\frac{\beta_n}{2}} \end{pmatrix} = \frac{x-L}{\sqrt{4t}}e^{-\frac{\boldsymbol{\beta}}{2}} \tag{33}$$

$$\boldsymbol{Y_0} = \begin{pmatrix} \frac{-L}{\sqrt{4t}}e^{-\frac{\beta_1}{2}} \\ \vdots \\ \frac{-L}{\sqrt{4t}}e^{-\frac{\beta_n}{2}} \end{pmatrix} = \frac{-L}{\sqrt{4t}}e^{-\frac{\boldsymbol{\beta}}{2}} \tag{34}$$

Define $\boldsymbol{E}$ and $\boldsymbol{E_0}$ as follows:

$$\boldsymbol{E} = \operatorname{erfc}(\boldsymbol{Y}) \tag{35}$$

$$\boldsymbol{E_0} = \operatorname{erfc}(\boldsymbol{Y_0}) \tag{36}$$

Therefore

$$E_{ratio} = diag(\boldsymbol{E}./\boldsymbol{E_0}) \tag{37}$$

Take the total differential of w:

$$\mathbf{d}\,\boldsymbol{w} = \mathbf{d}\,P \times E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)$$
$$+P \times \mathbf{d}\,E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)$$
$$+P \times E_{ratio} \times \mathbf{d}\,P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \tag{38}$$

According to Eq. (37)

$$\mathbf{d}\,E_{ratio} = \mathbf{d}\,diag(\boldsymbol{E}./\boldsymbol{E_0})$$
$$= diag\left(\mathbf{d}\,(\boldsymbol{E}./\boldsymbol{E_0})\right)$$
$$= diag\left({(\mathbf{d}\,\boldsymbol{E} \odot \boldsymbol{E_0} - \boldsymbol{E} \odot \mathbf{d}\,\boldsymbol{E_0}).} \Big/ {(\boldsymbol{E_0} \odot \boldsymbol{E_0})} \right) \tag{39}$$

To calculate $\mathbf{d}\,\boldsymbol{E}$:

$$\mathbf{d}\,\boldsymbol{E} = \mathbf{d}\,\mathrm{erfc}(\boldsymbol{Y}) = -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \mathbf{d}\,\boldsymbol{Y}$$
$$= -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \mathbf{d}\left(\frac{x-L}{\sqrt{4t}} e^{-\frac{\boldsymbol{\beta}}{2}}\right)$$
$$= -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot \left(\frac{x-L}{\sqrt{4t}} * (-\frac{1}{2}) * e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta} - \frac{1}{\sqrt{4t}}\, e^{-\frac{\boldsymbol{\beta}}{2}} \mathbf{d}\,L\right)$$
$$= \frac{x-L}{\sqrt{4\pi t}} e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta} + \frac{1}{\sqrt{\pi t}}\left(e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \mathbf{d}\,L$$
$$= \tfrac{x-L}{\sqrt{4\pi t}} dE \odot \mathbf{d}\,\boldsymbol{\beta} + \tfrac{1}{\sqrt{\pi t}} dE\ \mathbf{d}\,L \tag{40}$$

where

$$dE = e^{-\boldsymbol{Y}\odot\boldsymbol{Y}} \odot e^{-\frac{\boldsymbol{\beta}}{2}} \tag{41}$$

Likewise, to calculate $\mathbf{d}\,\boldsymbol{E}$:

$$\mathbf{d}\,\boldsymbol{E_0} = \mathbf{d}\,\mathrm{erfc}(\boldsymbol{Y_0}) = -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y_0}\odot\boldsymbol{Y_0}} \odot \mathbf{d}\,\boldsymbol{Y_0}$$
$$= -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y_0}\odot\boldsymbol{Y_0}} \odot \mathbf{d}\left(\frac{-L}{\sqrt{4t}} e^{-\frac{\boldsymbol{\beta}}{2}}\right)$$
$$= -\frac{2}{\sqrt{\pi}} e^{-\boldsymbol{Y_0}\odot\boldsymbol{Y_0}} \odot \left(\frac{-L}{\sqrt{4t}} * (-\frac{1}{2}) * e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta} - \frac{1}{\sqrt{4t}}\, e^{-\frac{\boldsymbol{\beta}}{2}} \mathbf{d}\,L\right)$$
$$= \frac{-L}{\sqrt{4\pi t}} e^{-\boldsymbol{Y_0}\odot\boldsymbol{Y_0}} \odot e^{-\frac{\boldsymbol{\beta}}{2}} \odot \mathbf{d}\,\boldsymbol{\beta} + \frac{1}{\sqrt{\pi t}}\left(e^{-\boldsymbol{Y_0}\odot\boldsymbol{Y_0}} \odot e^{-\frac{\boldsymbol{\beta}}{2}}\right) \mathbf{d}\,L$$

$$= \frac{-L}{\sqrt{4\pi t}} dE_0 \odot \mathbf{d}\,\boldsymbol{\beta} + \frac{1}{\sqrt{\pi t}} dE_0 \,\mathbf{d}\, L \tag{42}$$

where

$$dE_0 = e^{-\boldsymbol{Y_0} \odot \boldsymbol{Y_0}} \odot e^{-\frac{\boldsymbol{\beta}}{2}} \tag{43}$$

Plug Eq. (40) and Eq. (42) into Eq. (39), we have

$$\mathbf{d}\, E_{ratio} = diag\left((\mathbf{d}\, \boldsymbol{E} \odot \boldsymbol{E_0} - \boldsymbol{E} \odot \mathbf{d}\, \boldsymbol{E_0}) .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right)$$

$$= diag\left(\begin{pmatrix} \frac{x-L}{\sqrt{4\pi t}} dE \odot \mathbf{d}\,\boldsymbol{\beta} \odot \boldsymbol{E_0} + \frac{1}{\sqrt{\pi t}} (dE \odot \boldsymbol{E_0}) \mathbf{d}\, L \\ - \frac{-L}{\sqrt{4\pi t}} \boldsymbol{E} \odot dE_0 \odot \mathbf{d}\,\boldsymbol{\beta} - \frac{1}{\sqrt{\pi t}} (\boldsymbol{E} \odot dE_0) \mathbf{d}\, L \end{pmatrix} .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right)$$

$$= diag\left(\begin{pmatrix} \frac{x-L}{\sqrt{4\pi t}} dE \odot \boldsymbol{E_0} \odot \mathbf{d}\,\boldsymbol{\beta} + \frac{1}{\sqrt{\pi t}} (dE \odot \boldsymbol{E_0}) \mathbf{d}\, L \\ - \frac{-L}{\sqrt{4\pi t}} \boldsymbol{E} \odot dE_0 \odot \mathbf{d}\,\boldsymbol{\beta} - \frac{1}{\sqrt{\pi t}} (\boldsymbol{E} \odot dE_0) \mathbf{d}\, L \end{pmatrix} .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right)$$

$$= diag\left(\left(\frac{x-L}{\sqrt{4\pi t}} dE \odot \boldsymbol{E_0} + \frac{L}{\sqrt{4\pi t}} \boldsymbol{E} \odot dE_0 \right) .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right) \odot \mathbf{d}\, diag(\boldsymbol{\beta})$$

$$+ diag\left(\left(\frac{1}{\sqrt{\pi t}} dE \odot \boldsymbol{E_0} - \frac{1}{\sqrt{\pi t}} \boldsymbol{E} \odot dE_0 \right) .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right) \mathbf{d}\, L$$

$$= dE_{ratio1} \odot \mathbf{d}\, diag(\boldsymbol{\beta}) + dE_{ratio2} \mathbf{d}\, L \tag{44}$$

where

$$dE_{ratio1} = diag\left(\left(\frac{x-L}{\sqrt{4\pi t}} dE \odot \boldsymbol{E_0} + \frac{L}{\sqrt{4\pi t}} \boldsymbol{E} \odot dE_0 \right) .\!\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0}) \right) \tag{45}$$

and

$$dE_{ratio2} = diag\left(\left(\frac{1}{\sqrt{\pi t}} dE \odot \boldsymbol{E_0} - \frac{1}{\sqrt{\pi t}} \boldsymbol{E} \odot dE_0\right) .\Big/ (\boldsymbol{E_0} \odot \boldsymbol{E_0})\right) \tag{46}$$

To calculate $\mathbf{d}\, P^{-1}$,

$$\mathbf{d}\, P^{-1} = -P^{-1} \times \mathbf{d}\, P \times P^{-1} \tag{47}$$

Plug Eq. (44) and Eq. (47) into Eq. (38)

$$\begin{aligned} \mathbf{d}\, \boldsymbol{w} = \mathbf{d}\, P \times E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \\ + P \times \left(dE_{ratio1} \odot \mathbf{d}\, diag(\boldsymbol{\beta})\right) \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \\ + P \times dE_{ratio2} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \mathbf{d}\, L \\ - P \times E_{ratio} \times P^{-1} \times \mathbf{d}\, P \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right) \end{aligned} \tag{48}$$

Take the vectorization of each term of Eq. (48):

$$\begin{aligned} vec\left(\mathbf{d}\, P \times E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right) \\ = \left(\left(E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right)^T \otimes I_n\right) \times vec(dP) \end{aligned} \tag{49}$$

$$\begin{aligned} vec\left(P \times \left(dE_{ratio1} \odot \mathbf{d}\, diag(\boldsymbol{\beta})\right) \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right) \\ = \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right)^T \otimes P\right) \times vec\{dE_{ratio1} \odot \mathbf{d}\, diag(\boldsymbol{\beta})\} \\ = \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right)^T \otimes P\right) \times diag\left(vec(dE_{ratio1})\right) \times vec\left(\mathbf{d}\, diag(\boldsymbol{\beta})\right) \end{aligned} \tag{50}$$

and

$$\begin{aligned} vec\left(-P \times E_{ratio} \times P^{-1} \times \mathbf{d}\, P \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right) \\ = -\left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}}\right)\right)^T \otimes (P \times E_{ratio} \times P^{-1})\right) \times vec(dP) \end{aligned} \tag{51}$$

Therefore, the vectorization of $\mathbf{d}\, \boldsymbol{w}$ is

$$vec(dw) = \Bigg\{ \left(\left(E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \otimes I_n \right)$$

$$- \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \otimes (P \times E_{ratio} \times P^{-1}) \right) \Bigg\} \times vec(dP)$$

$$+ \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \otimes P \right) \times diag\left(vec(dE_{ratio1})\right) \times vec\left(\mathbf{d}\; diag(\boldsymbol{\beta})\right)$$

$$+ P \times dE_{ratio2} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \mathbf{d}\, L \tag{52}$$

Therefore,

$$w_L = \left(P \times dE_{ratio2} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \tag{53}$$

$$w_P = \frac{\partial w}{\partial P} = \Bigg\{ \left(\left(E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \otimes I_n \right)$$

$$- \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right)^T \otimes (P \times E_{ratio} \times P^{-1}) \right) \Bigg\}^T$$

$$= \left(\left(E_{ratio} \times P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right) \quad \otimes I_n \right)$$

$$- \left(\left[P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right] \quad \otimes \left[P \times E_{ratio} \times P^{-1} \right]^T \right) \tag{54}$$

$$w_{diag\,\boldsymbol{\beta}} = \frac{\partial w}{\partial diag\,\boldsymbol{\beta}} = diag\left(vec(dE_{ratio1})\right) \times \left(\left(P^{-1} \times \left(\boldsymbol{w_{interface}} - \boldsymbol{w_{initial}} \right) \right) \quad \otimes P^T \right) \tag{55}$$

To get $\frac{\partial w_{n+1}}{\partial L}$, $\frac{\partial w_{n+1}}{\partial P}$ and $\frac{\partial w_{n+1}}{\partial diag\,\boldsymbol{\beta}}$:

$$\frac{\partial w_{n+1}}{\partial L} = -\sum_i^n w_L\,(:,i) \tag{56}$$

$$\frac{\partial w_{n+1}}{\partial P} = -\sum_i^n w_P\,(:,i) \tag{57}$$

$$\frac{\partial w_{n+1}}{\partial diag\,\boldsymbol{\beta}} = -\sum_i^n w_{diag\,\boldsymbol{\beta}}\,(:,i) \tag{58}$$

Since $r = {}^{(w_0 - w \quad).}\!/_{\sigma}$, we have

$$r_L = {}^{-w_L \cdot}\!/_{\sigma} \tag{59}$$

$$r_P = {}^{-w_P \cdot}\!/_{\sigma} \tag{60}$$

$$r_{diag\ \boldsymbol{\beta}} = {}^{-w_{diag\ \boldsymbol{\beta}} \cdot}\!/_{\sigma} \tag{61}$$

And

$$\frac{\partial r_{n+1}}{\partial L} = {}^{\left(\sum_i^n w_L\,(:, i)\right)}\!\Big/_{\sigma_{n+1}} \tag{62}$$

$$\frac{\partial r_{n+1}}{\partial P} = {}^{\left(\sum_i^n w_P\,(:, i)\right)}\!\Big/_{\sigma_{n+1}} \tag{63}$$

$$\frac{\partial r_{n+1}}{\partial diag\ \boldsymbol{\beta}} = {}^{\left(\sum_i^n w_{diag\ \boldsymbol{\beta}}\,(:, i)\right)}\!\Big/_{\sigma_{n+1}} \tag{64}$$