Notes on time-domain analysis for terahertz spectroscopy

J. Steven Dodge[1,*]

[1] *Department of Physics, Simon Fraser University, Burnaby, BC, Canada*

I. PARAMETER ESTIMATION

Consider two N-dimensional vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ that satisfy $\boldsymbol{y} = \boldsymbol{H}(\boldsymbol{\theta})\boldsymbol{x}$, where $\boldsymbol{\theta}$ is an M-dimensional parameter vector for the transformation matrix $\boldsymbol{H}$. Let $\boldsymbol{x_m} = \boldsymbol{x} + \boldsymbol{\epsilon_x}$ and $\boldsymbol{y_m} = \boldsymbol{y} + \boldsymbol{\epsilon_y}$ be noisy measurements of these vectors, where $\boldsymbol{\epsilon_x}$ and $\boldsymbol{\epsilon_y}$ are N-dimensional vectors of $N(0,1)$ random variables with known covariance matrices $\boldsymbol{V_x}$ and $\boldsymbol{V_y}$. The negative-log-likelihood function is

$$-\log L(\mathbf{x},\mathbf{y},\boldsymbol{\theta}) = \frac{1}{2}\left[(\mathbf{x_m}-\mathbf{x})^{\intercal}\,\mathbf{V_x}^{-1}(\mathbf{x_m}-\mathbf{x}) + (\mathbf{y_m}-\mathbf{y})^{\intercal}\,\mathbf{V_y}^{-1}(\mathbf{y_m}-\mathbf{y})\right], \text{with } \mathbf{y} = \mathbf{H}(\boldsymbol{\theta})\mathbf{x}.$$

Assuming for simplicity that $\boldsymbol{V_x}$ and '$\boldsymbol{V_y}$ are diagnonal, and introducing an N-dimensional vector of Lagrange parameters $\boldsymbol{\lambda}$ to implement the constraints, we can define the maximum-likelihood cost function

$$K(\mathbf{x},\mathbf{y},\boldsymbol{\theta},\boldsymbol{\lambda}) = \sum_k \left\{\frac{(x_{mk}-x_k)^2}{2\sigma_{xk}^2} + \frac{(y_{mk}-y_k)^2}{2\sigma_{yk}^2} + \lambda_k\left[y_k - \sum_l H_{kl}(\boldsymbol{\theta})x_l\right]\right\},$$

and minimize with respect to $\boldsymbol{x}$, $\boldsymbol{y}$, $\boldsymbol{\theta}$, and $\boldsymbol{\lambda}$. The parameters of interest are $\boldsymbol{\theta}$; minimizing with respect to the remaining parameters gives the equations

$$\frac{\partial K}{\partial x_j} = -\frac{x_{mj}-x_j}{\sigma_{xj}^2} - \sum_k \lambda_k H_{kj}(\boldsymbol{\theta}) = 0, \tag{1}$$

$$\frac{\partial K}{\partial y_j} = -\frac{y_{mj}-y_j}{\sigma_{yj}^2} + \lambda_j = 0, \tag{2}$$

$$\frac{\partial K}{\partial \lambda_j} = y_j - \sum_l H_{jl}(\boldsymbol{\theta})x_l = 0, \tag{3}$$

$$\tag{4}$$

which we can use to eliminate the dependence of 'K on $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{\lambda}$. The algebra is given below.

$$y_j = \sum_l H_{jl}(\boldsymbol{\theta})x_l, \tag{5}$$

$$\lambda_j = \sigma_{yj}^{-2}(y_{mj}-y_j), \tag{6}$$

$$x_j = x_{mj} + \sigma_{xj}^2\sum_k \lambda_k H_{kj}(\boldsymbol{\theta}) \tag{7}$$

$$= x_{mj} + \sigma_{xj}^2\sum_k \sigma_{yk}^{-2}(y_{mk}-y_k)H_{kj}(\boldsymbol{\theta}) \tag{8}$$

$$= x_{mj} + \sigma_{xj}^2\sum_k \sigma_{yk}^{-2}\left[y_{mk} - \sum_l H_{kl}(\boldsymbol{\theta})x_l\right]H_{kj}(\boldsymbol{\theta}) \tag{9}$$

$$= x_{mj} + \sigma_{xj}^2\sum_k \sigma_{yk}^{-2}\left[y_{mk}H_{kj}(\boldsymbol{\theta}) - \sum_l H_{jk}^{\intercal}(\boldsymbol{\theta})H_{kl}(\boldsymbol{\theta})x_l\right], \tag{10}$$

$$\Rightarrow x_j + \sigma_{xj}^2\sum_{kl} H_{jk}^{\intercal}(\boldsymbol{\theta})\sigma_{yk}^{-2}H_{kl}(\boldsymbol{\theta})x_l = x_{mj} + \sigma_{xj}^2\sum_k y_{mk}\sigma_{yk}^{-2}H_{kj}(\boldsymbol{\theta}). \tag{11}$$

---

* jsdodge@sfu.ca

In vector notation, we have

$$\mathbf{y} = \mathbf{H}(\boldsymbol{\theta})\mathbf{x}, \tag{12}$$

$$\boldsymbol{\lambda} = \mathbf{V_y}^{-1}(\mathbf{y_m} - \mathbf{y}), \tag{13}$$

$$\mathbf{x} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\mathbf{x} = \mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m} \tag{14}$$

$$\Rightarrow \mathbf{x} = \left[\mathbf{1} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\right]^{-1}\left[\mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m}\right]. \tag{15}$$

Substituting for $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{\lambda}$ in K yields a new cost function, $K'(\boldsymbol{\theta})$, that involves only the parameters of interest:

$$K'(\boldsymbol{\theta}) = \frac{1}{2}\left\{\mathbf{x_m} - \left[\mathbf{1} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\right]^{-1}\left[\mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m}\right]\right\}^\intercal \times \tag{16}$$

$$\mathbf{V_x}^{-1}\left\{\mathbf{x_m} - \left[\mathbf{1} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\right]^{-1}\left[\mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m}\right]\right\} \tag{17}$$

$$+ \frac{1}{2}\left\{\mathbf{y_m} - \mathbf{H}(\boldsymbol{\theta})\left[\mathbf{1} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\right]^{-1}\left[\mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m}\right]\right\}^\intercal \times \tag{18}$$

$$\mathbf{V_y}^{-1}\left\{\mathbf{y_m} - \mathbf{H}(\boldsymbol{\theta})\left[\mathbf{1} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{H}(\boldsymbol{\theta})\right]^{-1}\left[\mathbf{x_m} + \mathbf{V_x}\mathbf{H}^\intercal(\boldsymbol{\theta})\mathbf{V_y}^{-1}\mathbf{y_m}\right]\right\}. \tag{19}$$

For a frequency-domain transmission amplitude function $t(\boldsymbol{\theta};\omega)$, the time-domain transfer matrix $\boldsymbol{H}(\boldsymbol{\theta})$ is

$$\mathbf{H}(\boldsymbol{\theta}) = \frac{1}{N}\boldsymbol{F}_N^\dagger \mathbf{t}(\boldsymbol{\theta};\boldsymbol{\omega})\boldsymbol{F}_N,$$

where $\boldsymbol{F}_N$ is the FFT matrix (generated for the $+i\omega t$ convention with `dftmtx` in `MATLAB`) and $t(\boldsymbol{\theta};\omega)$ is the diagonal matrix of the amplitude function evaluated at $\boldsymbol{\omega} = 2\pi\boldsymbol{F}$, where $\boldsymbol{f}$ is the vector of positive and negative frequencies associated with the N-dimensional FFT (see, for example, here).

II. NOISE MODEL

Consider M measurements of an unknown, band-limited signal $\mu(t)$ subject to amplitude drift and temporal drift, so that the signal associated with measurement $j = 0, 1, \ldots, M-1$ is

$$\zeta(t; A_j, \eta_j) = A_j\mu(t - \eta_j). \tag{20}$$

For each signal measurement we obtain N noisy samples at the nominal times $t_n = nT, n = 0, 1, \ldots, N-1$, which we arrange $N \times M$ matrix $\mathbf{x}$:

$$\begin{aligned} x_{ij} &= (1 + \beta_{ij})\zeta(t_i + \tau_{ij}; A_j, \eta_j) + \alpha_{ij} && (21)\\ &= A_j(1 + \beta_{ij})\mu(t_i - \eta_j + \tau_{ij}) + \alpha_{ij}, && (22)\end{aligned}$$

where the random variables $\alpha_{ij} \sim \mathcal{N}(0, \sigma_\alpha^2)$, $\beta_{ij} \sim \mathcal{N}(0, \sigma_\beta^2)$, and $\tau_{ij} \sim \mathcal{N}(0, \sigma_\tau^2)$ are fully independent and account for additive, multiplicative, and timebase noise, respectively. To fix the scale and location of $\mu(t)$, we set $(1/M)\sum A_j = 1$ and $\sum \eta_j = 0$, but otherwise make no assumptions about their distribution.

Expanding around the ideal value to first order in the random variables and introducing the notation, $\zeta_{ij} = \zeta(t_i; A_j, \eta_j)$ and $\dot{\zeta}_{ij} = \dot{\zeta}(t_i; A_j, \eta_j)$, gives

$$\begin{aligned} x_{ij} &\approx (1 + \beta_{ij})(\zeta_{ij} + \tau_{ij}\dot{\zeta}_{ij}) + \alpha_{ij} \\ &= \zeta_{ij} + \alpha_{ij} + \beta_{ij}\zeta_{ij} + \tau_{ij}\dot{\zeta}_{ij}. && (23)\end{aligned}$$

We can further relate ζ_{ij} and $\dot{\zeta}_{ij}$ to the ideal signal samples, $\mu_i = \mu(t_i)$ by defining the shift matrix $\mathbf{S}(\eta)$ and the derivative matrix $\mathbf{D}$, so that

$$\zeta_{ij} = A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)\mu_k, \tag{24}$$

$$\dot{\zeta}_{ij} = A_j \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\mu_l. \tag{25}$$

We can compute the matrix elements of $\mathbf{S}(\eta)$, $\mathbf{S}'(\eta)$, and $\mathbf{D}$, by recognizing that in general, a frequency-response function $H(\omega)$ can be represented in the time domain as transfer matrix $\mathbf{h}$,

$$h_{jk} = \frac{1}{N} \sum_{l=-(N-1)/2}^{(N-1)/2} H(\omega_l) e^{2\pi i(j-k)l/N} \tag{26}$$

where we let $\omega_l = 2\pi l/NT$, T is the sampling time, and we have assumed N to be odd (the trigonometric interpolation for even N yields a slightly different expression that I'll incorporate later).

This gives (in the $+i\omega t$ convention used by MATLAB)

$$S_{jk}(\eta) = \frac{1}{N} \sum_{l=-(N-1)/2}^{(N-1)/2} \exp(-i\omega_l\eta) e^{2\pi i(j-k)l/N}, \tag{27}$$

$$S'_{jk}(\eta) = \frac{1}{N} \sum_{l=-(N-1)/2}^{(N-1)/2} -i\omega_l \exp(-i\omega_l\eta) e^{2\pi i(j-k)l/N}, \text{ and} \tag{28}$$

$$D_{jk} = \frac{1}{N} \sum_{l=-(N-1)/2}^{(N-1)/2} i\omega_l e^{2\pi i(j-k)l/N}, \tag{29}$$

which we can all compute using the same (FFT) algorithm.

We get estimates $\hat{\boldsymbol{\mu}}$, $\widehat{\sigma_\alpha^2}$, $\widehat{\sigma_\beta^2}$, $\widehat{\sigma_\tau^2}$, $\hat{\mathbf{A}}$, and $\hat{\boldsymbol{\eta}}$ of the unknown parameters by maximizing the likelihood function,

$$\mathcal{L}(\mathbf{x}; \boldsymbol{\mu}, \sigma_\alpha^2, \sigma_\beta^2, \sigma_\tau^2, \mathbf{A}, \boldsymbol{\eta}) = \prod_{i,j} \left(2\pi\sigma_{ij}^2\right)^{-1/2} \exp\left[-\frac{(x_{ij}-\zeta_{ij})^2}{2\sigma_{ij}^2}\right], \tag{30}$$

with

$$\sigma_{ij}^2 = \sigma_\alpha^2 + \sigma_\beta^2\zeta_{ij}^2 + \sigma_\tau^2\dot{\zeta}_{ij}^2. \tag{31}$$

Alternatively, we may also minimize the negative log-likelihood cost function,

$$\begin{aligned} C(\mathbf{x}; \boldsymbol{\mu}, \sigma_\alpha^2, \sigma_\beta^2, \sigma_\tau^2, \mathbf{A}, \boldsymbol{\eta}) &= -\log \mathcal{L}(\mathbf{x}; \boldsymbol{\mu}, \sigma_\alpha^2, \sigma_\beta^2, \sigma_\tau^2, \mathbf{A}, \boldsymbol{\eta}) \\ &= \frac{MN}{2}\log(2\pi) + \frac{1}{2}\sum_{i,j}\log(\sigma_{ij}^2) + \frac{1}{2}\sum_{i,j}\frac{(x_{ij}-\zeta_{ij})^2}{\sigma_{ij}^2}, \end{aligned} \tag{32}$$

which is more computationally convenient.

To minimize C in practice, we use a trust-region reflective algorithm that relies on the function gradient, given analytically below.

$$\frac{\partial C}{\partial \mu_n} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial \mu_n} - \sum_{i,j}\frac{x_{ij}-\zeta_{ij}}{\sigma_{ij}^2}\frac{\partial \zeta_{ij}}{\partial \mu_n}, \tag{33a}$$

$$\frac{\partial C}{\partial \sigma_\alpha^2} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial \sigma_\alpha^2}, \tag{33b}$$

$$\frac{\partial C}{\partial \sigma_\beta^2} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial \sigma_\beta^2}, \tag{33c}$$

$$\frac{\partial C}{\partial \sigma_\tau^2} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial \sigma_\tau^2}, \tag{33d}$$

$$\frac{\partial C}{\partial A_m} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial A_m} - \sum_{i,j}\frac{x_{ij}-\zeta_{ij}}{\sigma_{ij}^2}\frac{\partial \zeta_{ij}}{\partial A_m}, \tag{33e}$$

$$\frac{\partial C}{\partial \eta_m} = \frac{1}{2}\sum_{i,j}\left[\frac{1}{\sigma_{ij}^2} - \frac{(x_{ij}-\zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}\right]\frac{\partial \sigma_{ij}^2}{\partial \eta_m} - \sum_{i,j}\frac{x_{ij}-\zeta_{ij}}{\sigma_{ij}^2}\frac{\partial \zeta_{ij}}{\partial \eta_m}. \tag{33f}$$

From Eq. 24,

$$\frac{\partial \zeta_{ij}}{\partial \mu_n} = \frac{\partial}{\partial \mu_n}\left[A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)\mu_k\right] = A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)\delta_{kn} = A_j S_{in}(\eta_j), \tag{34a}$$

$$\frac{\partial \zeta_{ij}}{\partial A_m} = \frac{\partial}{\partial A_m}\left[A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)\mu_k\right] = \delta_{jm} \sum_{k=0}^{N-1} S_{ik}(\eta_j)\mu_k = \delta_{jm}\frac{\zeta_{ij}}{A_j}, \quad \text{and} \tag{34b}$$

$$\frac{\partial \zeta_{ij}}{\partial \eta_m} = \frac{\partial}{\partial \eta_m}\left[A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)\mu_k\right] = \delta_{jm} A_j \sum_{k=0}^{N-1} S'_{ik}(\eta_j)\mu_k. \tag{34c}$$

From Eq. 25,

$$\frac{\partial \dot{\zeta}_{ij}}{\partial \mu_n} = \frac{\partial}{\partial \mu_n}\left[A_j \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\mu_l\right] = A_j \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\delta_{ln} = A_j \sum_{k=0}^{N-1} S_{ik}(\eta_j)D_{kn}, \tag{35a}$$

$$\frac{\partial \dot{\zeta}_{ij}}{\partial A_m} = \frac{\partial}{\partial A_m}\left[A_j \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\mu_l\right] = \delta_{jm} \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\mu_l = \delta_{jm}\frac{\dot{\zeta}_{ij}}{A_j}, \quad \text{and} \tag{35b}$$

$$\frac{\partial \dot{\zeta}_{ij}}{\partial \eta_m} = \frac{\partial}{\partial \eta_m}\left[A_j \sum_{k,l=0}^{N-1} S_{ik}(\eta_j)D_{kl}\mu_l\right] = \delta_{jm} A_j \sum_{k,l=0}^{N-1} S'_{ik}(\eta_j)D_{kl}\mu_l. \tag{35c}$$

From Eq. 31,

$$\frac{\partial \sigma_{ij}^2}{\partial \sigma_\alpha^2} = 1, \qquad \frac{\partial \sigma_{ij}^2}{\partial \sigma_\beta^2} = \zeta_{ij}^2, \qquad \text{and} \quad \frac{\partial \sigma_{ij}^2}{\partial \sigma_\tau^2} = \dot{\zeta}_{ij}^2. \tag{36}$$

Also from Eq. 31,

$$\frac{\partial \sigma_{ij}^2}{\partial \mu_n} = 2\sigma_\beta^2 \zeta_{ij}\frac{\partial \zeta_{ij}}{\partial \mu_n} + 2\sigma_\tau^2 \dot{\zeta}_{ij}\frac{\partial \dot{\zeta}_{ij}}{\partial \mu_n}, \tag{37a}$$

$$\frac{\partial \sigma_{ij}^2}{\partial A_m} = 2\sigma_\beta^2 \zeta_{ij}\frac{\partial \zeta_{ij}}{\partial A_m} + 2\sigma_\tau^2 \dot{\zeta}_{ij}\frac{\partial \dot{\zeta}_{ij}}{\partial A_m}, \quad \text{and} \tag{37b}$$

$$\frac{\partial \sigma_{ij}^2}{\partial \eta_m} = 2\sigma_\beta^2 \zeta_{ij}\frac{\partial \zeta_{ij}}{\partial \eta_m} + 2\sigma_\tau^2 \dot{\zeta}_{ij}\frac{\partial \dot{\zeta}_{ij}}{\partial \eta_m}. \tag{37c}$$

We can further simplify Eqs. 37 using Eqs. 34 and Eqs. 35,

$$\frac{\partial \sigma_{ij}^2}{\partial \mu_n} = 2A_j\left[\sigma_\beta^2 \zeta_{ij} S_{in}(\eta_j) + \sigma_\tau^2 \dot{\zeta}_{ij} \sum_{k=0}^{N-1} S_{ik}(\eta_j)D_{kn}\right], \tag{38a}$$

$$\frac{\partial \sigma_{ij}^2}{\partial A_m} = (2\delta_{jm}/A_m)(\sigma_\beta^2 \zeta_{im}^2 + \sigma_\tau^2 \dot{\zeta}_{im}^2), \quad \text{and} \tag{38b}$$

$$\frac{\partial \sigma_{ij}^2}{\partial \eta_m} = 2A_m\delta_{jm}\left[\sigma_\beta^2 \zeta_{im} \sum_{k=0}^{N-1} S'_{ik}(\eta_m)\mu_k + \sigma_\tau^2 \dot{\zeta}_{im} \sum_{k,l=0}^{N-1} S'_{ik}(\eta_m)D_{kl}\mu_l\right]. \tag{38c}$$

Substituting in Eqs. 33, we get

$$
\begin{aligned}
\frac{\partial C}{\partial \mu_n} &= \sum_{i,j} A_j \left\{ \left[\frac{\sigma_{ij}^2 - (x_{ij} - \zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2} \right] \left[\sigma_\beta^2 \zeta_{ij} S_{in}(\eta_j) + \sigma_\tau^2 \dot{\zeta}_{ij} \sum_{k=0}^{N-1} S_{ik}(\eta_j) D_{kn} \right] \right. \\
&\qquad \left. - \frac{x_{ij} - \zeta_{ij}}{\sigma_{ij}^2} S_{in}(\eta_j) \right\}, \qquad \text{(39a)} \\
\frac{\partial C}{\partial \sigma_\alpha^2} &= \frac{1}{2} \sum_{i,j} \frac{\sigma_{ij}^2 - (x_{ij} - \zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}, \qquad \text{(39b)} \\
\frac{\partial C}{\partial \sigma_\beta^2} &= \frac{1}{2} \sum_{i,j} \zeta_{ij}^2 \frac{\sigma_{ij}^2 - (x_{ij} - \zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}, \qquad \text{(39c)} \\
\frac{\partial C}{\partial \sigma_\tau^2} &= \frac{1}{2} \sum_{i,j} \dot{\zeta}_{ij}^2 \frac{\sigma_{ij}^2 - (x_{ij} - \zeta_{ij})^2}{\left(\sigma_{ij}^2\right)^2}, \qquad \text{(39d)} \\
\frac{\partial C}{\partial A_m} &= \frac{1}{A_m} \sum_i \left\{ (\sigma_\beta^2 \zeta_{im}^2 + \sigma_\tau^2 \dot{\zeta}_{im}^2) \left[\frac{\sigma_{im}^2 - (x_{im} - \zeta_{im})^2}{\left(\sigma_{im}^2\right)^2} \right] - \frac{x_{im} - \zeta_{im}}{\sigma_{im}^2} \zeta_{im} \right\}, \qquad \text{(39e)} \\
\frac{\partial C}{\partial \eta_m} &= A_m \left\{ \sum_i \left[\frac{\sigma_{im}^2 - (x_{im} - \zeta_{im})^2}{\left(\sigma_{im}^2\right)^2} \right] \left[\sigma_\beta^2 \zeta_{im} \sum_{k=0}^{N-1} S'_{ik}(\eta_m) \mu_k + \sigma_\tau^2 \dot{\zeta}_{im} \sum_{k,l=0}^{N-1} S'_{ik}(\eta_m) D_{kl} \mu_l \right] \right. \\
&\qquad \left. - \sum_{i,k} \frac{x_{im} - \zeta_{im}}{\sigma_{im}^2} S'_{ik}(\eta_m) \mu_k \right\}. \qquad \text{(39f)}
\end{aligned}
$$