

The **discretized energy** E can be expressed as:

$$E = \sum_{i=1}^J \sum_{\substack{j=1 \\ |j-i|>1}}^J k_{i,j} \|x_{i+1} - x_i\| \|x_{j+1} - x_j\| \quad (1)$$

$$k_{i,j} = \frac{1}{4} (k_{\beta}^{\alpha}(x_i, x_j, T_i) + k_{\beta}^{\alpha}(x_i, x_{j+1}, T_i) + k_{\beta}^{\alpha}(x_{i+1}, x_j, T_i) + k_{\beta}^{\alpha}(x_{i+1}, x_{j+1}, T_i)) \quad (2)$$

where we index cyclically.

For derivative with respect to x_k (note that it is a vector), the only terms indexed by (i, j) that involves x_k are enumerated by the following indices:

- $(k, 1), \dots, (k, k-2), (k, k+2), \dots, (k, J)$
- $(k-1, 1), \dots, (k-1, k-3), (k-1, k+1), \dots, (k-1, J)$
- $(1, k), \dots, (k-2, k), (k+2, k), \dots, (J, k)$
- $(1, k-1), \dots, (k-3, k-1), (k+1, k-1), \dots, (J, k-1)$

We now attempt to construct derivative (in a “modular fashion”). Write

$$\begin{aligned} k_{\beta}^{\alpha}(x_p, x_q, T_r) &= k_{\beta}^{\alpha}\left(x_p, x_q, \frac{x_{r+1} - x_r}{\|x_r - x_{r+1}\|}\right) \\ &= \frac{\sqrt{\|x_{r+1} - x_r\|^2 \|x_p - x_q\|^2 - ((x_{r+1} - x_r) \cdot (x_p - x_q))^2}^{\alpha}}{\|x_p - x_q\|^{\beta} \|x_r - x_{r+1}\|^{\alpha}} \\ &= \frac{\xi_{p,q,r}^{\alpha/2}}{\eta_{p,q,r}} \end{aligned} \quad (3)$$

where

$$\xi_{p,q,r} = \|x_{r+1} - x_r\|^2 \|x_p - x_q\|^2 - ((x_{r+1} - x_r) \cdot (x_p - x_q))^2 \quad (4)$$

$$\eta_{p,q,r} = \|x_p - x_q\|^{\beta} \|x_r - x_{r+1}\|^{\alpha} \quad (5)$$

Derivative with respect to x_k can now be written as:

$$\frac{\partial}{\partial x_k} \left(\frac{\xi^{\alpha/2}}{\eta} \right) = \frac{1}{\eta^2} \left(\frac{\alpha}{2} \xi^{\alpha/2-1} \frac{\partial \xi}{\partial x_k} \eta - \xi^{\alpha/2} \frac{\partial \eta}{\partial x_k} \right) \quad (6)$$

where p, q, r are omitted.

$$\mathbf{1} \quad (p, q, r) = (k, j, k)$$

$$\xi_{k,j,k} = \|x_{k+1} - x_k\|^2 \|x_k - x_j\|^2 - ((x_{k+1} - x_k) \cdot (x_k - x_j))^2 \quad (7)$$

$$\eta_{k,j,k} = \|x_k - x_j\|^{\beta} \|x_k - x_{k+1}\|^{\alpha} \quad (8)$$

Taking derivative of $\xi_{k,j,k}$ with respect to x_k ,

$$\frac{\partial \xi_{k,j,k}}{\partial x_k} = 2(x_k - x_{k+1}) \|x_k - x_j\|^2 \quad (9)$$

$$+ 2\|x_{k+1} - x_k\|^2 (x_k - x_j) \quad (10)$$

$$- 2(x_{k+1} - x_k) \cdot (x_k - x_j) (x_j + x_{k+1} - 2x_k) \quad (11)$$

Taking derivative of $\eta_{k,j,k}$ with respect to x_k ,

$$\frac{\partial \eta_{k,j,k}}{\partial x_k} = \beta \|x_k - x_j\|^{\beta-2} \|x_k - x_{k+1}\|^\alpha (x_k - x_j) \quad (12)$$

$$+ \alpha \|x_k - x_j\|^\beta \|x_k - x_{k+1}\|^{\alpha-2} (x_k - x_{k+1}) \quad (13)$$

2 $(p, q, r) = (i, j, k)$ where $i \neq k$ or $i \neq k - 1$

$$\xi_{i,j,k} = \|x_{k+1} - x_k\|^2 \|x_i - x_j\|^2 - ((x_{k+1} - x_k) \cdot (x_i - x_j))^2 \quad (14)$$

$$\eta_{i,j,k} = \|x_i - x_j\|^\beta \|x_k - x_{k+1}\|^\alpha \quad (15)$$

Taking derivative of $\xi_{i,j,k}$ with respect to x_k ,

$$\frac{\partial \xi_{i,j,k}}{\partial x_k} = 2\|x_i - x_j\|^2 (x_k - x_{k+1}) \quad (16)$$

$$- 2(x_{k+1} - x_k) \cdot (x_i - x_j) (x_j - x_i) \quad (17)$$

Taking derivative of $\eta_{i,j,k}$ with respect to x_k ,

$$\frac{\partial \eta_{i,j,k}}{\partial x_k} = \alpha \|x_i - x_j\|^\beta \|x_k - x_{k+1}\|^{\alpha-2} (x_k - x_{k+1}) \quad (18)$$

3 $(p, q, r) = (k - 1, j, k - 1)$

$$\xi_{k-1,j,k-1} = \|x_k - x_{k-1}\|^2 \|x_{k-1} - x_j\|^2 - ((x_k - x_{k-1}) \cdot (x_{k-1} - x_j))^2 \quad (19)$$

$$\eta_{k-1,j,k-1} = \|x_{k-1} - x_j\|^\beta \|x_{k-1} - x_k\|^\alpha \quad (20)$$

Taking derivative of $\xi_{k-1,j,k-1}$ with respect to x_k ,

$$\frac{\partial \xi_{k-1,j,k-1}}{\partial x_k} = 2\|x_{k-1} - x_j\|^2 (x_k - x_{k-1}) \quad (21)$$

$$- 2(x_k - x_{k-1}) \cdot (x_{k-1} - x_j) (x_{k-1} - x_j) \quad (22)$$

Taking derivative of $\eta_{k-1,j,k-1}$ with respect to x_k ,

$$\frac{\partial \eta_{k-1,j,k-1}}{\partial x_k} = \alpha \|x_{k-1} - x_j\|^\beta \|x_k - x_{k-1}\|^{\alpha-2} (x_k - x_{k-1}) \quad (23)$$

$$4 \quad (p, q, r) = (k, j, k-1)$$

$$\xi_{k,j,k-1} = \|x_k - x_{k-1}\|^2 \|x_k - x_j\|^2 - ((x_k - x_{k-1}) \cdot (x_k - x_j))^2 \quad (24)$$

$$\eta_{k,j,k-1} = \|x_k - x_j\|^\beta \|x_{k-1} - x_k\|^\alpha \quad (25)$$

Taking derivative of $\xi_{k,j,k-1}$ with respect to x_k ,

$$\frac{\partial \xi_{k,j,k-1}}{\partial x_k} = 2\|x_k - x_j\|^2 (x_k - x_{k-1}) \quad (26)$$

$$+ 2\|x_k - x_{k-1}\|^2 (x_k - x_j) \quad (27)$$

$$- 2(x_k - x_{k-1}) \cdot (x_k - x_j) (2x_k - x_j - x_{k-1}) \quad (28)$$

Taking derivative of $\eta_{k,j,k-1}$ with respect to x_k ,

$$\frac{\partial \eta_{k,j,k-1}}{\partial x_k} = \beta \|x_{k-1} - x_k\|^\alpha \|x_k - x_j\|^{\beta-2} (x_k - x_j) \quad (29)$$

$$+ \alpha \|x_k - x_j\|^\beta \|x_k - x_{k-1}\|^{\alpha-2} (x_k - x_{k-1}) \quad (30)$$

$$5 \quad (p, q, r) = (j, k, j)$$

$$\xi_{j,k,j} = \|x_{j+1} - x_j\|^2 \|x_k - x_j\|^2 - ((x_{j+1} - x_j) \cdot (x_k - x_j))^2 \quad (31)$$

$$\eta_{j,k,j} = \|x_k - x_j\|^\beta \|x_j - x_{j+1}\|^\alpha \quad (32)$$

Taking derivative of $\xi_{j,k,j}$ with respect to x_k ,

$$\frac{\partial \xi_{j,k,j}}{\partial x_k} = 2\|x_{j+1} - x_j\|^2 (x_k - x_j) \quad (33)$$

$$- 2(x_{j+1} - x_j) \cdot (x_k - x_j) (x_{j+1} - x_j) \quad (34)$$

Taking derivative of $\eta_{j,k,j}$ with respect to x_k ,

$$\frac{\partial \eta_{j,k,j}}{\partial x_k} = \beta \|x_j - x_{j+1}\|^\alpha \|x_k - x_j\|^{\beta-2} (x_k - x_j) \quad (35)$$