

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  $x_k$ ,

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