calculation of root mean square difference

real number data , a_x and b_x

$$\begin{cases} a_x & \text{with } x = 0, \cdots, N_a - 1 \\ b_x & \text{with } x = 0, \cdots, N_b - 1 \end{cases}$$

displacement of b_x with respect to a_x , d

$$d = D_1, \cdots, D_2 \quad \text{where } 1 - N_b \le D_1 \le D_2 \le N_a - 1$$

number of overlapped data , $O(d)$

$$O(d) = \begin{cases} \left.\begin{matrix} N_b + d & \text{when } 1 - N_b \le d \le 0 \\ N_b & \text{when } 0 \le d \le N_a - N_b \\ N_a - d & \text{when } N_a - N_b \le d \le N_a - 1 \end{matrix}\right\} \text{when } N_a \ge N_b \\ \hline \left.\begin{matrix} N_b + d & \text{when } 1 - N_b \le d \le N_a - N_b \\ N_a & \text{when } N_a - N_b \le d \le 0 \\ N_a - d & \text{when } 0 \le d \le N_a - 1 \end{matrix}\right\} \text{when } N_a \le N_b \end{cases}$$

sum of squared data , $SS(d)$

$$SS(d) = \sum_{x=0}^{O(d)-1} \begin{cases} (a_x^2 + b_{x-d}^2) & \text{when } d \le 0 \\ (a_{x+d}^2 + b_x^2) & \text{when } d \ge 0 \end{cases}$$

cross correlation of data , $CC(d)$

$$CC(d) = \sum_{x=0}^{O(d)-1} \begin{cases} a_x \cdot b_{x-d} & \text{when } d \le 0 \\ a_{x+d} \cdot b_x & \text{when } d \ge 0 \end{cases}$$

mean square difference of data , $MSD(d)$

$$MSD(d) = \frac{1}{O(d)} \cdot \sum_{x=0}^{O(d)-1} \begin{cases} (a_x - b_{x-d})^2 & \text{when } d \le 0 \\ (a_{x+d} - b_x)^2 & \text{when } d \ge 0 \end{cases}$$

$$= \frac{SS(d) - 2 \cdot CC(d)}{O(d)}$$

root mean square difference of data , $RMSD(d)$

$$RMSD(d) = \sqrt{MSD(d)} \quad \text{for } d = D_1, \cdots, D_2$$

calculation of $SS(d)$ and $CC(d)$ using discrete Fourier transform (DFT)

number of terms for DFT , M

$$M > \max(N_a, N_b) + \max(| D_1 |, | D_2 |) \quad \rightarrow \text{ if } d = 1 - N_b, \cdots, N_a - 1 \text{ then } M \ge 2 \cdot \max(N_a, N_b)$$

calculation of $SS(d)$

[SS1] for $x = 0, \cdots, M-1$ set $g_x = \begin{cases} a_x^2 & \text{when } x < N_a \\ 0 & \text{when } x \ge N_a \end{cases} + i \cdot \begin{cases} b_x^2 & \text{when } x < N_b \\ 0 & \text{when } x \ge N_b \end{cases}$

[SS2] for $u = 0, \cdots, M-1$ set $G_u = \sum_{x=0}^{M-1} g_x \cdot \exp(- i \cdot 2 \cdot \pi \cdot x \cdot u / M)$ ← DFT

[SS3] set $p_0 = \mathrm{Re}(G_0) \cdot N_b + N_a \cdot \mathrm{Im}(G_0)$

for $u = 1, \cdots, M-1$

set $\alpha_u = \exp(- i \cdot \pi \cdot (N_a - 1) \cdot u / M) \cdot \sin(\pi \cdot N_a \cdot u / M) / \sin(\pi \cdot u / M)$

$\beta_u = \exp(+ i \cdot \pi \cdot (N_b - 1) \cdot u / M) \cdot \sin(\pi \cdot N_b \cdot u / M) / \sin(\pi \cdot u / M)$

$p_u = \frac{1}{2} \cdot \left((G_u + G_{M-u}^*) \cdot \beta_u + i \cdot \alpha_u \cdot (G_u^* - G_{M-u}) \right)$

[SS4] for $x = 0, \cdots, M-1$ set $P_x = \sum_{u=0}^{M-1} p_u \cdot \exp(+ i \cdot 2 \cdot \pi \cdot u \cdot x / M)$ ← inverse DFT

[SS5] $SS(d) = \frac{1}{M} \cdot \begin{cases} \mathrm{Re}(P_{M+d}) & \text{when } d < 0 \\ \mathrm{Re}(P_d) & \text{when } d \ge 0 \end{cases}$

calculation of $CC(d)$

[CC1] for $x = 0, \cdots, M-1$ set $h_x = \begin{cases} a_x & \text{when } x < N_a \\ 0 & \text{when } x \ge N_a \end{cases} + i \cdot \begin{cases} b_x & \text{when } x < N_b \\ 0 & \text{when } x \ge N_b \end{cases}$

[CC2] for $u = 0, \cdots, M-1$ set $H_u = \sum_{x=0}^{M-1} h_x \cdot \exp(- i \cdot 2 \cdot \pi \cdot x \cdot u / M)$ ← DFT

[CC3] set $q_0 = \mathrm{Re}(H_0) \cdot \mathrm{Im}(H_0)$

for $u = 1, \cdots, M-1$ set $q_u = i \cdot \frac{1}{4} \cdot (H_u + H_{M-u}^*) \cdot (H_u^* - H_{M-u})$

[CC4] for $x = 0, \cdots, M-1$ set $Q_x = \sum_{u=0}^{M-1} q_u \cdot \exp(+ i \cdot 2 \cdot \pi \cdot u \cdot x / M)$ ← inverse DFT

[CC5] $CC(d) = \frac{1}{M} \cdot \begin{cases} \mathrm{Re}(Q_{M+d}) & \text{when } d < 0 \\ \mathrm{Re}(Q_d) & \text{when } d \ge 0 \end{cases}$