1 Positive Definiteness of the cgDNA stiffness matrix and Invariance of the parameter set

Let $\mathcal{P} = \left\{K^{\alpha\beta}, \sigma^{\alpha\beta}, K^{\alpha}, \sigma^{\alpha} | \alpha\beta \in D \text{ and } \alpha \in M\right\}$ be a cgDNA parameter set where D is the set of all dimers (two base pairs) formed using $M = \{A, T, C, G\}$, and let $S = X_1, X_2, \ldots, X_n$ be a sequence with $X_i \in \{A, T, C, G\}$

1. Assume that

$$K^{\alpha\beta} + \frac{1}{2}\begin{bmatrix} K^{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & K^{\beta} \end{bmatrix} > 0, \tag{1}$$

$$K^{\alpha\beta} + \begin{bmatrix} K^{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}K^{\beta} \end{bmatrix} > 0, \tag{2}$$

$$K^{\alpha\beta} + \begin{bmatrix} \frac{1}{2}K^{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & K^{\beta} \end{bmatrix} > 0, \tag{3}$$

for all $K^{\alpha\beta}$, K^{α}, and K^{β} in $\mathcal{P}$. Show that the cgDNA stiffness matrix $K(S, \mathcal{P})$ is positive definite for any sequence S.

2. Define by E_{2m-1} the trailing-diagonal matrix with $2m-1$ repetitions of $E = diag(-1, 1, 1, -1, 1, 1)$, and define by $\overline{S}$ the complementary sequence of S. By assuming

$$\begin{aligned} K^{\overline{\alpha\beta}} &= E_3 K^{\alpha\beta} E_3, \\ \sigma^{\overline{\alpha\beta}} &= E_3 \sigma^{\alpha\beta}, \\ K^{\overline{\alpha}} &= E K^{\alpha} E, \\ \sigma^{\overline{\alpha}} &= E \sigma^{\alpha}, \end{aligned}$$

where $\overline{\beta}\overline{\alpha}$ and $\overline{\alpha}$ are the complementaries sequence to, respectively, $\alpha\beta$ and α, show that for any sequence S:

$$\begin{aligned} K(\overline{S}, \mathcal{P}) &= E_{2n-1} K(S, \mathcal{P}) E_{2n-1}, \\ \mu(\overline{S}, \mathcal{P}) &= E_{2n-1} \mu(S, \mathcal{P}), \end{aligned}$$

so that $\rho(\overline{\mathbf{w}}; \overline{S}, \mathcal{P}) = \rho(\mathbf{w}; S, \mathcal{P})$, where $\overline{\mathbf{w}} = E_{2n-1}\mathbf{w}$.

3. Using part 2), how many of the conditions in part 1) are independent?

2 Zero entries in the cgDNA parameter set

i) Describe all of the restrictions on the cgDNA parameters $K^{\alpha\overline{\alpha}}, \sigma^{\alpha\overline{\alpha}}$, and $\hat{x}^{\alpha\overline{\alpha}}$ for each of the palindromic dimer steps $\alpha\overline{\alpha}$, $\alpha \in \{A, T, C, G\}$.

ii) If S is a palindromic sequence, i.e., $\overline{S} = S$, what are the corresponding restrictions on the reconstructions, $K(S), \sigma(S)$, $\mu(S)$.

3 Total number of unknowns in a cgDNA parameter set

Let $\mathcal{P} = \left\{K^{\alpha\beta}, \sigma^{\alpha\beta}, K^{\alpha}, \sigma^{\alpha} | \alpha\beta \in D \text{ and } \alpha \in M\right\}$, where D is the set of all dimers formed using the alphabet $M = \{A, T, G, C\}$, be a cgDNA parameter set. Using all the symmetry conditions (i.e. Crick-Watson symmetries (Ex. 1) and palindrome restrictions (Ex. 2)) find the total number of independent scalars in the parameter set $\mathcal{P}$.

4 Square roots in SE(3)

In the cgDNA model we have defined the basepair frame as the mid frame between two base frames by using the usual square root for the rotation part and the euclidean average for the $\mathbb{R}^3$ part. The latter way of defining the mid frame is also used to define the junction frames between two consecutive basepair frames. In this exercise we will study the difference between the cgDNA way of defining the mid frames and the square root in SE(3) which could be used as alternative way for the representation of the a mid frame. Let $G \in SE(3)$, then

$$G = \begin{bmatrix} Q & q \\ 0_3^T & 1 \end{bmatrix}, \tag{4}$$

where $Q \in SO(3)$, $q \in \mathbb{R}^3$. Let $B \in SE(3)$ such that

$$B = \begin{bmatrix} Q^{\frac{1}{2}} & x \\ 0_3^T & 1 \end{bmatrix}. \tag{5}$$

Find x such that $BB = G$. What can you say about B.