Inferring 3D chromatin structure using a multiscale approach based on quaternions Supplementary Material

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Here we report an essential account on basic characteristics of quaternions. Further details on quaternion algebra can be found in [35]. Let us consider the following extended concept of a complex number:

$$\mathbf{q} = q_0 + q_1 i + q_2 j + q_3 k \tag{1}$$

where q_0, q_1, q_2 and q_3 are real numbers, and the imaginary units i, j and k obey the following fundamental formulas, which define the product of quaternions

$$\begin{aligned} i^2 = j^2 = k^2 = -1 \\ ij = -ji = k \\ jk = -kj = i \\ ki = -ik = j \end{aligned} \tag{2}$$

If $q_0 = 0$, $\mathbf{q}$ is called a *pure quaternion*, and is the analogous of an $\mathbb{R}^3$ vector $(q_0, q_1, q_2)^T$. The conjugate, norm, and inverse of $\mathbf{q}$, respectively, are defined as

$$\bar{\mathbf{q}} = q_0 - q_1 i - q_2 j - q_3 k \tag{3}$$

$$||\mathbf{q}|| = \sqrt{\bar{\mathbf{q}}\mathbf{q}} = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2} \tag{4}$$

$$\mathbf{q}^{-1} = \frac{\bar{\mathbf{q}}}{||\mathbf{q}||^2} \tag{5}$$

Quaternions with $||\mathbf{q}|| = 1$ are called *unit quaternions*. Unlike real or complex products, the product of quaternions is not commutative. The rotation of a vector $(v_x, v_y, v_z)^T$, represented as the pure quaternion $\mathbf{v} = v_x i + v_y j + v_z k$, of an angle θ around a direction identified by the unit pure quaternion $\mathbf{u} = (u_x, u_y, u_z)^T$, can be expressed through the map $\mathbf{v} \rightarrow \mathbf{R_q}(\mathbf{v}) = \mathbf{q}\mathbf{v}\bar{\mathbf{q}}$, where $\mathbf{q}$ is the unit quaternion

$$\mathbf{q} = cos\frac{\theta}{2} + sin\frac{\theta}{2}u_x i + sin\frac{\theta}{2}u_y j + sin\frac{\theta}{2}u_z k \tag{6}$$

The composition of two rotations is simply obtained through the product of the corresponding quaternions: $\mathbf{R_p}(\mathbf{R_q}(\mathbf{v})) = \mathbf{R_{pq}}(\mathbf{v})$. Note that, as the quaternion product is non-commutative, it is $\mathbf{R_{pq}} \neq \mathbf{R_{qp}}$. Also, since quaternions $\mathbf{q}$ and $-\mathbf{q}$ give the same rotation (changing the sign of $\mathbf{q}$ is increasing θ of 2π), it is $\mathbf{R_q} = \mathbf{R_{-q}}$.