Mathematical Functions of Lipid Repositioning Algorithm

1 Distance Function

Purpose: Calculate Euclidean distance between two points in 3D space.

Definition:

$$d(\mathbf{a}_1, \mathbf{a}_2) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$$

Where:

- $\mathbf{a}_1 = (x_1, y_1, z_1)$ – First atom position
- $\mathbf{a}_2 = (x_2, y_2, z_2)$ – Second atom position

2 Direction Vector Function

Purpose: Calculate direction vector from root to child atom.

Definition:

$$\vec{d}(\text{root}, \text{child}) = \text{child} - \text{root} = (x_c - x_r, y_c - y_r, z_c - z_r)$$

Where:

- root $= (x_r, y_r, z_r)$
- child $= (x_c, y_c, z_c)$

3 Vector Normalization Function

Purpose: Convert vector to unit vector.

Definition:

$$\hat{u} = \frac{\vec{v}}{|\vec{v}|} = \frac{\vec{v}}{\sqrt{v_x^2 + v_y^2 + v_z^2}}$$

Where $\vec{v} = (v_x, v_y, v_z)$.

4 Dot Product Function

Purpose: Compute scalar product of two vectors.

Definition:

$$\vec{a} \cdot \vec{b} = a_x b_x + a_y b_y + a_z b_z = |\vec{a}||\vec{b}| \cos\theta$$

Where θ is the angle between $\vec{a}$ and $\vec{b}$.

5 Cross Product Function

Purpose: Compute vector perpendicular to two input vectors.

Definition:

$$\vec{a} \times \vec{b} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = (a_y b_z - a_z b_y)\hat{i} - (a_x b_z - a_z b_x)\hat{j} + (a_x b_y - a_y b_x)\hat{k}$$

6 Rotation Matrix (Rodrigues' Formula)

Purpose: Create 3×3 rotation matrix to rotate from one vector to another.

Case 1: Vectors are identical ($\theta = 0°$)

$$R = I_{3\times 3} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Case 2: Vectors are opposite ($\theta = 180°$)

$$R = 2K^2 - I_{3\times 3}$$

Where K is the skew-symmetric matrix of the perpendicular axis.

Case 3: General case ($0° < \theta < 180°$)

Rodrigues' formula:

$$R = I + \sin\theta[\vec{k}]_\times + (1 - \cos\theta)[\vec{k}]_\times^2$$

Where:

- I = Identity matrix
- $\theta = \cos^{-1}(\hat{u} \cdot \hat{v})$
- $\vec{k} = \frac{\hat{u}\times\hat{v}}{|\hat{u}\times\hat{v}|}$
- $[\vec{k}]_\times$ is the skew-symmetric matrix of $\vec{k} = (k_x, k_y, k_z)$:

$$[\vec{k}]_\times = \begin{bmatrix} 0 & -k_z & k_y \\ k_z & 0 & -k_x \\ -k_y & k_x & 0 \end{bmatrix}$$

Expanded:

$$R = \begin{bmatrix} \cos\theta + k_x^2(1-\cos\theta) & k_x k_y(1-\cos\theta) - k_z\sin\theta & k_x k_z(1-\cos\theta) + k_y\sin\theta \\ k_y k_x(1-\cos\theta) + k_z\sin\theta & \cos\theta + k_y^2(1-\cos\theta) & k_y k_z(1-\cos\theta) - k_x\sin\theta \\ k_z k_x(1-\cos\theta) - k_y\sin\theta & k_z k_y(1-\cos\theta) + k_x\sin\theta & \cos\theta + k_z^2(1-\cos\theta) \end{bmatrix}$$

7 Atom Rotation Function

Purpose: Rotate atom coordinates around a pivot point using rotation matrix.
Definition:

$$\vec{P}_{\text{new}} = R(\vec{P}_{\text{old}} - \vec{P}_{\text{pivot}}) + \vec{P}_{\text{pivot}}$$

Steps:

1. Translate to origin: $\vec{P}_{\text{temp}} = \vec{P}_{\text{old}} - \vec{P}_{\text{pivot}}$
2. Rotate: $\vec{P}_{\text{rotated}} = R \cdot \vec{P}_{\text{temp}}$
3. Translate back: $\vec{P}_{\text{new}} = \vec{P}_{\text{rotated}} + \vec{P}_{\text{pivot}}$

8 Average Direction Function

Purpose: Compute mean direction from root to multiple tail atoms.
Definition:

$$\vec{d}_{\text{avg}} = \frac{1}{n} \sum_{i=1}^{n} \vec{d}(\text{root}, \text{tail}_i)$$

9 Residue Grouping Function

Purpose: Group atoms by residue ID.
Definition:

$$G : A \to \mathcal{P}(A), \quad G(\text{atoms}) = \{R_i \mid R_i = \{a \in A \mid a.\text{resID} = i\}\}$$

10 Root Finding Function

Purpose: Select anchor atom for each residue.
Definition:

$$\text{root}(R) = \begin{cases} \underset{a \in R}{\text{argmax}}(\text{'P'} \in a.\text{atomName}) & \text{if } \exists a \in R : \text{'P'} \in a.\text{atomName} \\ R[0] & \text{otherwise} \end{cases}$$

11 Distance-Based Sorting Function

Purpose: Select k atoms farthest from the root.
Definition:

$$\text{tails}(R, \text{root}, k) = \{a_i \mid a_i \in \text{sort}(R, \text{key} = \lambda a : d(a, \text{root}), \text{reverse=True})[:k]\}$$

12 Overall Algorithm Flow

Function Composition:

Lipid_Reposition = WriteFile∘RotateAllAtoms∘CreateRotationMatrix∘CalculateDirections∘GroupByResidue∘ReadFile