1 More properties of the Cayley transform

We will need two further results on the Cayley transformation. The inverse Cayley transform of $Q \in SO(3)$ is S was introduced in session 3. Now we define

$$u = Cay(Q) \Leftrightarrow [u\times] = (Q+\mathbf{I})^{-1}(Q-\mathbf{I}),$$

where $u \in \mathbb{R}^3$ and $Q \in SO(3)$. The function $Cay : SO(3) \to R^3$, $u = Cay(Q)$, is the mapping defined by u being the vector corresponding to the skew matrix $[u\times]$ that is the inverse Cayley transform of the rotation matrix Q. Prove that:

1. $Cay(Q^T) = -Cay(Q)$.

2. $Cay(P^TQP) = |P|P^T Cay(Q)$, $\forall P \in O(3)$.

3. Let $R, Q \in SO(3)$. Then $RQ = \bar{Q}R$ with $\bar{Q} = RQR^T \in SO(3)$. Show that the Cayley vectors $u = Cay(Q)$ of Q and $\bar{u} = Cay(\bar{Q})$ of $\bar{Q}$ are related by $\bar{u} = Ru$.

2 The change of reading strand transformation

2.1 Proof of the change of reading strand transformation Part-1

In the lecture we have discussed the *change of reading strand* transformation. We now prove a general result for two rigid bodies which includes an additional constant rotation P on one of the bodies. Later we will focus on the extension to the DNA, and more precisely we will derive the change of variable needed for the change of reading strand transformation for chains of rigid bodies. Let $(R,r)^-$ and $(R,r)^+$ be two frames and recall the following notation:

i) the Cayley vector of the relative rotation from "minus" to "plus" on the right : $u = Cay([R^-]^T R^+) \in \mathbb{R}^3$

ii) the mid frame (R,r): $R = R^-([R^-]^T R^+)^{\frac{1}{2}}$, $r = \dfrac{1}{2}(r^- + r^+)$

iii) the relative translation expressed in the mid frame: $v = R^T(r^+ - r^-) \in \mathbb{R}^3$

Let now $P \in O(3)$ and define

$$\overline{R}^{\pm} = R^{\mp} P.$$

Find the transformation of coordinates

$$u \mapsto \overline{u} \qquad (1)$$

$$v \mapsto \overline{v}, \qquad (2)$$

where $\overline{u}, \overline{v} \in \mathbb{R}^3$ are the internal coordinate between the pair of rigid bodies $(\overline{R}, \overline{r})^{\pm}$. Note that the transformation $R \to \overline{R}$, a) rotates by P and b) switches the role of $\pm$. You will also need to use Qn. 3.1 below at one step.

3 More on square roots of matrices (for completeness generalising the case $M \in SO(3)$)

3.1 On the general power of diagonalizable matrices

First we define the general power of a diagonalizable matrix (which includes the case of interest to us, $M \in SO(3)$):

Definition 1. *Let $M \in \mathbb{R}^{3\times3}$, be a diagonalisable matrix, so that there exists a matrix $R \in \mathbb{R}^{3\times3}$ or $\mathbb{C}^{3\times3}$, such that $M = RDR^{-1}$, with $D = diag(\lambda_1, \lambda_2, \lambda_3)$. The generalised power of M is denoted by M^α, $\alpha \in \mathbb{R}$, and is defined as*

$$M^\alpha = RD^\alpha R^{-1} \tag{3}$$

where

$$D^\alpha = diag(\lambda_1^\alpha, \lambda_2^\alpha, \lambda_3^\alpha). \tag{4}$$

Note that if

- $\alpha = -1$, M^α is the inverse of M,
- $\alpha = \frac{1}{2}$, M^α is the principal square root of M provided that $\lambda_i^{1/2}$ is taken as the principal square root of the complex number λ_i (see wikipedia).

By applying Definition (1) to a matrix $Q \in SO(3)$ we have that

$$Q^{\frac{1}{2}} = H diag\left(\exp\left(i\frac{\theta}{2}\right), \exp\left(-i\frac{\theta}{2}\right), 1\right)H^*, \text{ } H \text{ is hermitian, and } HH^* = \mathrm{I},$$

where $0 \leq \theta < \pi$ is the rotation angle of Q. Let now $P \in O(3)$ and $M \in \mathbb{R}^{3\times3}$ a diagonalizable matrix, prove that

$$(P^T MP)^\alpha = P^T M^\alpha P, \ \forall \alpha \in \mathbb{R}. \tag{5}$$

$\big[$ Note: for the case $\alpha \in \mathbb{N}$ there is no need to use the Definition (1)]

3.2 Square roots in SE(3)

In the cgDNA model we will define 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 is an alternative for the representation of a "mid" frame. But for our purposes the cgDNA way is simpler.
Let $G \in SE(3)$, then

$$G = \begin{bmatrix} Q & q \\ 0_3^T & 1 \end{bmatrix}, \tag{6}$$

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

$$B = \begin{bmatrix} \mathbf{X} & \mathbf{x} \\ 0_3^T & 1 \end{bmatrix}. \tag{7}$$

Find $\mathbf{X}$ and $\mathbf{x}$ such that $BB = G$, is $B = G^{1/2}$.

4 Review of various Matrix Factorisations (based on Linear Algebra courses you have followed, or wikipedia)

A brief summary on different factorisations are provided in the PDF linked to the description of lecture detail in week 4. Most or indeed all of the factorisations should be familiar to you. In particular we will later use the Cholesky factorisation of a symmetric positive definite matrix (in our Monte Carlo code) and the polar decomposition (in fitting frames to atomistic data).