Mathematical Modelling of DNA
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Session 4: Solutions — A. Patelli, R. Singh

1 More properties of the Cayley transform

For what follows, $P \in O(3)$ and $Q \in SO(3)$.

1. Define $\overline{u} := Cay(Q^T)$, as before we remark that $(Q^T \pm \mathbf{I}) = (Q \pm \mathbf{I})^T$. Thus, we obtain

$$[\overline{u}\times] = (Q+\mathbf{I})^{-T}(Q-\mathbf{I})^T = [(Q+\mathbf{I})^{-1}(Q-\mathbf{I})]^T = [u\times]^T = -[u\times]. \tag{1}$$

We used the fact that $(Q+\mathbf{I})^{-1}$ and $(Q-\mathbf{I})$ commute. Finally we obtain that

$$Cay(Q^T) = \overline{u} = -u = -Cay(Q). \tag{2}$$

2. Again define $\overline{u} := Cay(P^TQP)$, from the definition on the exercise sheet we obtain that

$$[\overline{u}\times] = (P^TQP+\mathbf{I})^{-1}(P^TQP-\mathbf{I}) \tag{3}$$

Since $P^TP = \mathbf{I}$ we have that $(P^TQP \pm \mathbf{I}) = P^T(Q \pm \mathbf{I})P$. Moreover $(P^T(Q\pm\mathbf{I})P)^{-1} = P^T(Q \pm \mathbf{I})^{-1}P$, thus we obtain that

$$[\overline{u}\times] = P^T(Q+\mathbf{I})^{-1}(Q-\mathbf{I})P = P^T[u\times]P = [|P|P^Tu\times], \tag{4}$$

where the last step uses Qn. 1.2 of Session 2. This implies

$$Cay(P^TQP) = \overline{u} = |P|P^Tu = |P|P^TCay(Q). \tag{5}$$

3. Again we can write

$$\begin{aligned} Cay(\bar{Q}) = Cay(RQR^T) &= R\ [u\times]\ R^T && \text{(using property 2 from above)} \\ &= [|R|\ R\ u\times] && \text{(using Qn. 1.2 of Session 2)} \\ &= R\ Cay(Q) && (|R| = 1) \end{aligned} \tag{6}$$

which implies $\bar{u} = R\ u$.

2 The change of reading strand transformation

2.1 Proof of the change of reading strand transformation Part I

Let $(R,r)^-$ and $(R,r)^+$ be two frames and recall the following notion:

- the Cayley vector of the relative rotation from "minus" to "plus" : $u = Cay([R^-]^TR^+) \in \mathbb{R}^3$
- the mid frame (R,r): $R = R^-([R^-]^TR^+)^{\frac{1}{2}}$, $r = \frac{1}{2}(r^- + r^+)$
- the relative translation: $v = R^T(r^+ - r^-) \in \mathbb{R}^3$,

Define now the analogous u and v but for the frames $(\overline{R},\overline{r})^{\pm}$ by $\overline{u}$ and $\overline{v}$,and let $P \in O(3)$. We want now to find the transformation between the Cayley vectors $\overline{u}$ and u:

$$\begin{aligned}
\overline{u} &= Cay([\overline{R}^-]^T\overline{R}^+) = Cay(P^T[R^+]^T R^- P) &(7)\\
&= |P|P^T Cay([R^+]^T R^-) = |P|P^T Cay(\big[[R^-]^T R^+\big]^T) &(8)\\
&= -|P|P^T Cay([R^-]^T R^+) = -|P|P^T u &(9)
\end{aligned}$$

Notice that we used the convention that the transformation is always from − to + but $\overline{R}^- = R^+P$ and $\overline{R}^+ = R^-P$. Before computing the transformation between the translational coordinates $\overline{v}$ and v we observe that the mid frame (R,r) can also be defined as the mid rotation from "plus" to "minus". In fact

$$\begin{aligned}
[R^-([R^-]^T R^+)^{\frac{1}{2}}]^T R^+([R^+]^T R^-)^{\frac{1}{2}} &= ([R^-]^T R^+)^{\frac{T}{2}}[R^-]^T R^+([R^+]^T R^-)^{\frac{1}{2}}\\
&= ([R^-]^T R^+)^{\frac{T}{2}}([R^-]^T R^+)^{\frac{1}{2}}([R^-]^T R^+)^{\frac{1}{2}}([R^+]^T R^-)^{\frac{1}{2}}\\
&= ([R^-]^T R^+)^{\frac{1}{2}}([R^+]^T R^-)^{\frac{1}{2}}\\
&= ([R^-]^T R^+)^{\frac{1}{2}}([R^-]^T R^+)^{\frac{T}{2}}\\
&= I,
\end{aligned}$$

thus $R = R^-([R^-]^T R^+)^{\frac{1}{2}} = R^+([R^+]^T R^-)^{\frac{1}{2}}$. Now we can compute the mid frame $(\overline{R},\overline{r})$:

$$\begin{aligned}
\overline{R} &= \overline{R}^-([\overline{R}^-]^T\overline{R}^+)^{\frac{1}{2}} = R^+P(P^T[R^+]^T R^- P)^{\frac{1}{2}}\\
&= R^+([R^+]^T R^-)^{\frac{1}{2}}P = RP
\end{aligned}$$

Thus we can find the transformation from $\overline{v}$ and v:

$$\overline{v} = \overline{R}^T(\overline{r}^+ - \overline{r}^-) = P^T R^T(r^- - r^+) = -P^T R^T(r^+ - r^-) = -P^T v \tag{10}$$

3 More on square roots of matrices

3.1 On the general power of diagonalizable matrices

Let $P \in O(3)$ and $M \in \mathbb{R}^{3\times3}$ a diagonalizable matrix , with $R \in \mathbb{F}^{3\times3}$ such that $M = RDR^{-1}$, $D = diag(\lambda_1,\lambda_2,\lambda_3)$.
We remark that $(P^TMP)^2 = (P^TMP)(P^TMP) = P^TMPP^TMP) = P^TM^2P$, because $P^TP = I$. Thus we have that for any power $\alpha \in \mathbb{N}$ we have

$$(P^TMP)^\alpha = (P^TMP)(P^TMP)\cdots(P^TMP) = P^TM^\alpha P.$$

Let $\alpha \in \mathbb{R}\setminus\mathbb{N}$ and let us use the decomposition $M = RDR^{-1}$. We obtain that $P^TMP = P^TRDR^{-1}P$. Define $\tilde{R} = P^TR$ thus, $P^TMP = \tilde{R}D\tilde{R}^{-1} = \tilde{M}$. Now, $\tilde{M} \in \mathbb{R}^{3\times3}$ is diagonalizable. Thus, we can apply the Definition 1 of the exercise sheet to obtain the generalized power $\tilde{M}^\alpha$,i.e,

$$(P^TMP)^\alpha = \tilde{M}^\alpha = \tilde{R}D^\alpha\tilde{R}^{-1} = P^TRD^\alpha R^{-1}P = P^TM^\alpha P. \tag{11}$$

The statement is proven.

3.2 Square roots in SE(3)

Using a direct computation one can easily find that

$$B = \begin{bmatrix} Q^{\frac{1}{2}} & (I+Q^{\frac{1}{2}})^{-1}q \\ 0_3^T & 1 \end{bmatrix}. \tag{12}$$

The transformation rules for this definition of mid-frame are much more complicated than those in (1-2) for the other choice of mid-frame.