1 Scaling of the Cayley transform

1. Let $u \in \mathbb{R}^3$ and $\alpha \in \mathbb{R}$ with $\alpha \neq 0$. We have that

$$Cay\left(\frac{1}{\alpha}[u \times]\right) = I + \frac{2}{1 + \frac{1}{\alpha}||u||^2}\left(\left[\frac{1}{\alpha}u \times\right] + \left[\frac{1}{\alpha}u \times\right]^2\right)$$
$$= I + \frac{2\alpha^2}{\alpha^2 + ||u||^2}\frac{1}{\alpha}\left([u \times] + [u \times]^2\right)$$
$$= I + \frac{2\alpha}{\alpha^2 + ||u||^2}\left([u \times] + \frac{1}{\alpha}[u \times]^2\right). \quad (1)$$

2. If the relation between $Q \in SO(3)$ and $u$ is known, for any $\alpha \in \mathbb{R}$, $\alpha \neq 0$ we can define

$$Cay^{-1}(Q) = \frac{\alpha}{(1 + tr(Q))}\left(Q - Q^T\right) = [\alpha u \times], \quad (2)$$

which implies that

$$||Cay^{-1}(Q)|| = \alpha \tan\left(\frac{\phi}{2}\right) = ||\alpha u||. \quad (3)$$

3. The routine `cay` in the function `frames.m` should be changed as follow:

```matlab
function [Q] = cay(u)
I = eye(3) ;
alpha = 10 ;
X = [ 0 -u(3) u(2) ; u(3) 0 -u(1) ; -u(2) u(1) 0 ] ;
Q = I + 2*alpha/(alpha^2 + norm(u)^2)*(X + 1/alpha*X^2) ;
end
```

2 Connection between the Cayley transform and the matrix exponential

1. Let $N \in \mathbb{R}^{n \times n}$ and $(I - N)$ invertible. We recall the Neumann expansion

$$(I - N)^{-1} = I + N + N^2 + N^3 + \ldots \quad (4)$$

The Cayley transformation of $N$ with a factor $\frac{1}{2}$ can be rewritten as

$$Cay\left(\frac{1}{2}N\right) = \left(I + \frac{1}{2}N\right)\left(I - \frac{1}{2}N\right)^{-1}$$
$$= \left(I + \frac{1}{2}N\right)\left(I + \frac{1}{2}N + \frac{1}{4}N^2 + \frac{1}{8}N^3 + \ldots\right)$$
$$= I + N + \frac{1}{2}N^2 + \frac{1}{4}N^3 + \ldots \quad (5)$$
The definition of the matrix exponential of \( N \) is given by the following Taylor expansion

\[
\exp(N) = I + \frac{1}{2}N + \frac{1}{4}N^2 + \frac{1}{8}N^3 + \ldots
\]  

(6)

Using (5) and (6) we obtain that

\[
\exp(N) - Cay \left( \frac{1}{2}N \right) = -\frac{1}{2}N^3 + \mathcal{O}(\|O\|^4).
\]

(7)

Thus for a matrix \( N \) with \( \|N\| \ll 1 \) we obtain that

\[
\exp(N) \approx Cay \left( \frac{1}{2}N \right)
\]

(8)

2. Let \( \mathbf{w} \in \mathbb{R}^3 \) and define the skew symmetric matrix \( N = [\mathbf{w} \times] \). We recall that the characteristic polynomial for \( N \) is \( \chi_N = -\|\mathbf{w}\|^2 N = \omega N \), where \( \omega := \|\mathbf{w}\| \). This implies that, \( N^{2m+1} = (-1)^m \omega^{2m} N \) and \( N^{2m} = (-1)^{m-1} \omega^{2m-2} N^2 \). Therefore,

\[
\exp(N) = \sum_{n=0}^{\infty} \frac{1}{n!} N^n = I + \sum_{m=0}^{\infty} \frac{1}{(2m+1)!} N^{2m+1} + \sum_{m=0}^{\infty} \frac{1}{(2m)!} N^{2m}
\]

\[
= I + \sum_{m=0}^{\infty} \frac{(-1)^m \omega^{2m}}{(2m+1)!} N + \sum_{m=1}^{\infty} \frac{(-1)^{m-1} \omega^{2m-2}}{(2m)!} N^2
\]

\[
= I + \sum_{m=0}^{\infty} \frac{(-1)^m \omega^{2m+1}}{(2m+1)!} N + \sum_{m=1}^{\infty} \frac{(-1)^{m-1} \omega^{2m-2}}{(2m)!} N^2
\]

\[
= I + \frac{1}{\omega} \sum_{m=0}^{\infty} \frac{(-1)^m \omega^{2m+1}}{(2m+1)!} N - \frac{1}{\omega^2} \sum_{m=1}^{\infty} \frac{(-1)^m \omega^{2m}}{(2m)!} N^2
\]

\[
= I + \frac{\sin \omega}{\omega} N + \frac{1 - \cos \omega}{\omega^2} N^2
\]

\[
= I + \frac{\|\mathbf{w}\|}{\|\mathbf{w}\|^2} \left[ \mathbf{w} \times \right] + \frac{1 - \cos \|\mathbf{w}\|}{\|\mathbf{w}\|^2} \left[ \mathbf{w} \times \right]^2.
\]

3. We can observe that if \( \bar{e} = \frac{\mathbf{w}}{\|\mathbf{w}\|} \) and \( \theta = \|\mathbf{w}\| \) we obtain that

\[
\exp([\mathbf{w} \times]) = I + \sin(\theta)[\bar{e} \times] + (1 - \cos(\theta))[\bar{e} \times]^2
\]

\[
= R(\theta, \bar{e})
\]

where is the Euler–Rodigures formula for a rotation around the unitary axis \( \bar{e} \) through an angle \( \theta \). Thus we obtain that for any \( \theta \in \mathbb{R} \) and any unitary vector \( \bar{e} \in \mathbb{R}^3 \) we have that \( \exp([\theta \bar{e} \times]) = R(\theta, \bar{e}) \in SO(3) \).

4. Let \( \mathbf{w} \in \mathbb{R}^3 \) with \( \|\mathbf{w}\| = \theta < \pi \). We have that \( \exp([\mathbf{w} \times]) = R(\theta, \bar{e}) \equiv R \) where \( \bar{e} = \frac{\mathbf{w}}{\theta} \). By direct computation we have

\[
(R - R^T) = \sin(\theta)[\bar{e} \times] = \frac{\sin(\theta)}{\theta} \left[ \mathbf{w} \times \right]
\]

\[
\frac{\theta}{\sin(\theta)}(R - R^T) = \left[ \mathbf{w} \times \right].
\]
Figure 1: Values of the differences in the helical parameters between ground-state of S₁ and ground-state of S₂.

3 Effect of a point mutation on the Shape and on the Stiffness

For questions 1-4 is useful to compute the difference $dx = x_1 - x_2$, where $x_i$ is the ground-state of sequence $S_i$. In Figure 1 we show the values of the helical parameters of $dx$.

In Figure 2 we show, using the command spy, the difference $dK = K_1 - K_2$, where $K_i$ is the stiffness matrix for sequence $S_i$. As already done in session 4 exercise 4.1.2, a point mutation leads to a local change in stiffness.

4 Proof of the change of reading strand transformation Part–2

The DNA fragment (with sequence $S = X_1, X_2, \ldots, X_N$) we are considering is described by the internal coordinates

$$x = ((\eta_1, w_1), (u_1, v_1), \ldots, (u_{N-1}, v_{N-1}), (\eta_N, w_N)) = (y_1, z_1, \ldots, z_{N-1}, y_N),$$

where $y_i = (\eta_i, w_i) \in \mathbb{R}^6$ are the intra base-pair variable and $z_l = (u_l, v_l) \in \mathbb{R}^6$ are the inter base-pair variables.

We first write down the base-pair frames and junction frames associated to $\{(R_i, r_i)^C, (R_i, r_i)^W\}_{i=1}^N$.

Define the $i$–th base-pair frame

For all $i = 1, 2, \ldots, N$:

- $R_i = R_i^C([R_i^C]^T R_i^W)^{\frac{1}{2}}$
- $r_i = \frac{1}{2}(r_i^C + r_i^W)$
Define the \( l \)-th junction frame

For all \( l = 1, 2, \ldots, N - 1 \):

- \( J_l = R_l(R_l^T R_{l+1})^{\frac{1}{2}} \)
- \( j_l = \frac{1}{2}(r_l + r_{l+1}) \)

For the change of reading strand transformation the matrix \( P \in O(3) \) we have to chose is

\[
P = \begin{bmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & -1
\end{bmatrix}.
\]

The next step is to identify the frames of the starting configuration with the frames of the transformed one. It is easy to see that the relation between the two configuration is:

\[
\begin{align*}
\overline{R}_{N+1-i}^C &= R_i^W P, & \overline{r}_{N+1-i}^C &= r_i^W \\
\overline{R}_{N+1-i}^W &= R_i^C P, & \overline{r}_{N+1-i}^W &= r_i^C \\
\overline{R}_{N+1-i} &= R_l P, & \overline{r}_{N+1-i} &= r_l \\
\overline{J}_{N-l} &= J_l P, & \overline{J}_{N-l} &= j_l.
\end{align*}
\]  

(9)

Define now the two linear transformation of the indices: \( \sigma(i) = N + 1 - i \) and \( \gamma(l) = N - l \). By using Exercise 1.2, serie 4, we can define the internal coordinate of the transformed configuration:
Inter variables
\[
\forall l = 1, \ldots, N - 1 \begin{cases} \bar{\eta}_\gamma(l) = -P^T u_l \\ \bar{\eta}_\gamma(l) = -P^T v_l \end{cases} \Rightarrow \bar{\eta}_\gamma(l) = \text{diag}(-P^T, -P^T)z_l = Ez_l.
\]
Here for each \( l \) we used the Exercise 4.1 with \( \{(R_l, r_l), (J_l, j_l), (R_{l+1}, r_{l+1})\} \) and the transformation \( P \).

Intra variables
\[
\forall i = 1, \ldots, N \begin{cases} \bar{\eta}_\sigma(i) = -P^T \eta_i \\ \bar{\eta}_\sigma(i) = -P^T w_i \end{cases} \Rightarrow \bar{\eta}_\sigma(i) = \text{diag}(-P^T, -P^T)y_i = Ey_i.
\]
Here for each \( i \) we used the Exercise 4.1 with \( \{(R_i^C, r_i^C), (R_i, r_i), (R_i^W, r_i^W)\} \) and the transformation \( P \).

Finally the change of reading strand transformation implies a change also on the sequence of the transformed DNA, i.e, \( \bar{S} = \bar{X}_N, \bar{X}_{N-1}, \ldots, \bar{X}_1 \). Now, the internal coordinates of the DNA fragment with sequence \( \bar{S} \) is described by
\[
\bar{x} = (\bar{y}_1, \bar{z}_1, \ldots, \bar{z}_{N-1}, \bar{y}_N)
\]
Using the indices transformation \( \sigma \) and \( \gamma \), and the relation on the inter and intra variables, we can rewrite \( \bar{x} \) as
\[
\bar{x} = (Ey_N, E\bar{z}_{N-1}, Ey_{N-1}, E\bar{z}_{N-2}, \ldots, E\bar{z}_1, Ey_1) = \begin{bmatrix} E & E & & & y_1 \\ & E & & & \vdots \\ & & \ddots & & \\ & & & E & \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_{N-1} \\ \bar{z}_1 \\ \bar{y}_N \end{bmatrix}
\]

5 On the symmetry of the coordinates system

Useful matlab function for this exercise:

1. The complementary sequence of \( S \) is \( \bar{S} = GCTTTTTTTTTCAC \). For checking that \( x(S) = E_n x(\bar{S}) \) one can compute \( \|x(S) - E_n x(\bar{S})\| \). While for the stiffness one can use the command \( \text{spy} \) in order to visualize the difference \( dK = K(S) - E_n K(\bar{S}) E_n \). Be aware that the command \( \text{spy} \) shows all non zero entries of the matrix or vector passed as argument. In order to filter out small entries one can use the following trick: \( \text{spy}( \text{abs}(dK) > 1e-10 ) \).

2. The sequence \( S \) is a palindrome which means that \( S = \bar{S} \). This implies the following:
   \[
   x(S) = E_n x(\bar{S}) = E_n x(S), \quad K(S) = E_n K(\bar{S}) E_n = E_n K(S) E_n.
   \]

From the above equation for the stiffness matrix \( K \), and by using the first part of this question, we can conclude that \( K(S) - E_n K(S) E_n \) is the zeros matrix. Finally in order to understand why the Shift in junction 6 is zero it is important to understand what happen to \( x(S) \) when multiplied by \( E_n \). More precisely what happen to the intras and the inters of \( x(S) \) See also the solution of the exercise 4.2 of this sheet. There will be an exercise later on in the semester where we will better explore the action of the matrix \( E_n \) on the ground-state and on the stiffness of palindromic sequences.