

Constant for

$$\|A - B\|_F^2 = \underbrace{\| \Lambda_A - \Lambda_B \|_F^2}_{\text{min of perm}}$$

$$\text{and } -\|A - B\|_F^2 + \underbrace{\| \Lambda_A - \Lambda_B \|_F^2}_{\text{max of perm}}$$

The $O(\Theta^2)$ term is

$$C = (\text{tr}(K^2 \Lambda_A \Lambda_B) - \text{tr}(K \Lambda_A K \Lambda_B))$$

(1) Exact computation of the constant is possible if we choose a (Λ_A, Q_A) and (Λ_B, Q_B) ordering. This in turn decides

$$Rot = (Q_A)^T Q_B$$

Then using Rodrigues formula

$$Rot = \exp(\Theta \underline{K})$$

with

$$Rot^T = Rot^{-1}, \det(Rot) = 1$$

and choosing $\|\underline{K}\| = 1$

will force

$$\|\underline{K}\|_F^2 = 2$$

The ordering of (Λ_A, Q_A) , (Λ_B, Q_B) will determine

Rot and this in turn will determine Θ and \underline{K} .

Question :-

How can we estimate C ?

(1) We would prefer not to determine C exactly since this will require first finding Q_A and Q_B which defeats the point of using the metric in the first place.

What do we know about K and K^2 ?

$$K = \begin{pmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{pmatrix} = -K^T$$

$$K^2 = \begin{pmatrix} -(k_3^2 + k_2^2) & k_2 k_1 & k_3 k_1 \\ k_2 k_1 & -(k_3^2 + k_1^2) & k_3 k_2 \\ k_3 k_1 & k_3 k_2 & -(k_2^2 + k_1^2) \end{pmatrix} = (K^2)^T$$

$$\begin{aligned} K^2 \Lambda_A \Lambda_B &= \begin{pmatrix} -\Lambda_{11}^B (k_3^2 + k_2^2) & \Lambda_{22}^B k_2 k_1 & \Lambda_{33}^B k_3 k_1 \\ \Lambda_{11}^B k_2 k_1 & -\Lambda_{22}^B (k_3^2 + k_1^2) & \Lambda_{33}^B k_3 k_2 \\ \Lambda_{11}^B k_3 k_1 & \Lambda_{22}^B k_3 k_2 & -\Lambda_{33}^B (k_2^2 + k_1^2) \end{pmatrix} \Lambda_A \\ &= \begin{pmatrix} -\Lambda_{11}^B \Lambda_{11}^A (k_3^2 + k_2^2) & \Lambda_{22}^A \Lambda_{22}^B k_2 k_1 & \Lambda_{33}^A \Lambda_{33}^B k_3 k_1 \\ \Lambda_{11}^A \Lambda_{11}^B k_2 k_1 & -\Lambda_{22}^A \Lambda_{22}^B (k_3^2 + k_1^2) & \Lambda_{33}^A \Lambda_{33}^B k_3 k_2 \\ \Lambda_{11}^A \Lambda_{11}^B k_3 k_1 & \Lambda_{22}^A \Lambda_{22}^B k_3 k_2 & -\Lambda_{33}^A \Lambda_{33}^B (k_2^2 + k_1^2) \end{pmatrix} \end{aligned}$$

$$\text{tr}(K^2 \Lambda_B \Lambda_A)$$

$$= -\Lambda_{11}^B \Lambda_{11}^A \underbrace{(k_3^2 + k_2^2)}_{1 - k_1^2} - \Lambda_{22}^A \Lambda_{22}^B \underbrace{(k_3^2 + k_1^2)}_{1 - k_2^2} + \Lambda_{33}^A \Lambda_{33}^B \underbrace{(k_2^2 + k_1^2)}_{1 - k_3^2}$$

$$\begin{aligned} &= -\Lambda_{11}^A \Lambda_{11}^B - \Lambda_{22}^A \Lambda_{22}^B - \Lambda_{33}^A \Lambda_{33}^B \\ &\quad + (\Lambda_{11}^A \Lambda_{11}^B k_1^2 + \Lambda_{22}^A \Lambda_{22}^B k_2^2 + \Lambda_{33}^A \Lambda_{33}^B k_3^2) \end{aligned}$$

Thus

$$\hbar(K^2 \Lambda_A \Lambda_A) - \hbar(K \Lambda_A K \Lambda_B)$$

$$= -\Lambda_{11}^A \Lambda_{11}^B (k_3^2 + k_2^2) - \Lambda_{22}^A \Lambda_{22}^B (k_3^2 + k_1^2) \\ - \Lambda_{33}^A \Lambda_{33}^B (k_2^2 + k_1^2)$$

$$+ k_3^2 \Lambda_{22}^A \Lambda_{11}^B + k_2^2 \Lambda_{33}^A \Lambda_{11}^B + k_3^2 \Lambda_{11}^A \Lambda_{22}^B + k_1^2 \Lambda_{33}^A \Lambda_{22}^B \\ + k_2^2 \Lambda_{11}^A \Lambda_{33}^B + k_1^2 \Lambda_{22}^A \Lambda_{33}^B$$

Making the approximation $k_1^2 = k_2^2 = k_3^2 = 1$

$$\text{then } \hbar(K^2 \Lambda_B \Lambda_A) - \hbar(K \Lambda_A K \Lambda_B)$$

$$= -2\Lambda_{11}^A \Lambda_{11}^B - \Lambda_{22}^A \Lambda_{22}^B - \Lambda_{33}^A \Lambda_{33}^B \\ + \Lambda_{22}^A \Lambda_{11}^B + \Lambda_{33}^A \Lambda_{11}^B + \Lambda_{11}^A \Lambda_{22}^B + \Lambda_{33}^A \Lambda_{22}^B + \Lambda_{11}^A \Lambda_{33}^B \\ + \Lambda_{22}^A \Lambda_{33}^B$$