1 Gaussian Integral III

Let define $f_{X,Y}(x,y)$ the joint distribution of the two random variables X and Y. The distribution of X given that Y is fixed to a value y, can be written as

$$f_X(x|Y=y) = \frac{f_{X,Y}(x,y)}{f_Y(y)}, \tag{1}$$

where $f_Y(y)$ is the marginal distribution for Y. In the case of Gaussian distribution we can explicitly compute the latter ratio and find a close form for the conditional distribution. The main idea is to decompose the quadratic form in the argument of the exponential into the marginal plus the conditional. This computation has already been done in the solution of the Exercise 2 serie 13 where we aimed at computing the marginal distribution of a Gaussian. Here we propose a similar decomposition than the one presented in the solution of the Exercise 2 serie 13:

$$(\mathbf{x}-\hat{\mathbf{x}})\cdot K(\mathbf{x}-\hat{\mathbf{x}}) = (\mathbf{x}_2-\hat{\mathbf{x}}_2)\cdot \Sigma_{22}^{-1}(\mathbf{x}_2-\hat{\mathbf{x}}_2) + (\mathbf{x}_1-(\hat{\mathbf{x}}_1+\eta))\cdot K_{11}(\mathbf{x}_1-(\hat{\mathbf{x}}_1+\eta)), \tag{2}$$

where $\Sigma_{22}^{-1} = K_{22} - K_{12}^T K_{11}^{-1} K_{12}$ and $\eta = -K_{11}^{-1}K_{12}(\mathbf{x}_2-\hat{\mathbf{x}}_2)$. By using the first result obtained in the solution of Exercise 2 serie 13 one can define the blocks of K in term of the blocks of Σ, and one can find that $K_{11} = (\Sigma_{11} - \Sigma_{21}^T\Sigma_{22}^{-1}\Sigma_{21})^{-1}$, and that $\eta = \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{x}_2-\hat{\mathbf{x}}_2)$. Finally by defining :

$$f(\mathbf{x}) = f(\mathbf{x}_1,\mathbf{x}_2) = \frac{1}{Z}\exp\left\{-\frac{1}{2}(\mathbf{x}-\hat{\mathbf{x}})\cdot K(\mathbf{x}-\hat{\mathbf{x}})\right\}, \tag{3}$$

$$f_2(\mathbf{x}_2) = \frac{1}{Z_2}\exp\left\{-\frac{1}{2}(\mathbf{x}_2-\hat{\mathbf{x}}_2)\cdot \Sigma_{22}^{-1}(\mathbf{x}_2-\hat{\mathbf{x}}_2)\right\}, \tag{4}$$

We obtain that

$$f(\mathbf{x}_1|\mathbf{x}_2=a) = \frac{f(\mathbf{x}_1,\mathbf{a})}{f_2(\mathbf{a})} = \frac{1}{\overline{\overline{Z}}}\exp\left\{-\frac{1}{2}(\mathbf{x}_1-\overline{\mathbf{x}})\cdot \overline{\Sigma}^{-1}(\mathbf{x}_1-\overline{\mathbf{x}})\right\}, \tag{5}$$

where $\overline{\mathbf{x}} = \hat{\mathbf{x}}_1 + \Sigma_{12}\Sigma_{22}^{-1}(\mathbf{a}-\hat{\mathbf{x}}_2), \overline{\Sigma}^{-1} = K_{11}$.

2 On the computation of conditionals of the cgDNA+ probability distribution

In Figure 1 and Figure 2 we show the cgDNA+ groundstate (in red) and computed conditional groundstate (in blue) when a constrains/condition (see in the question) is applied to a particular Watson phosphate. One can notice the non local change in the value of groundstate coordinates due to the condition on one of the phosphate.

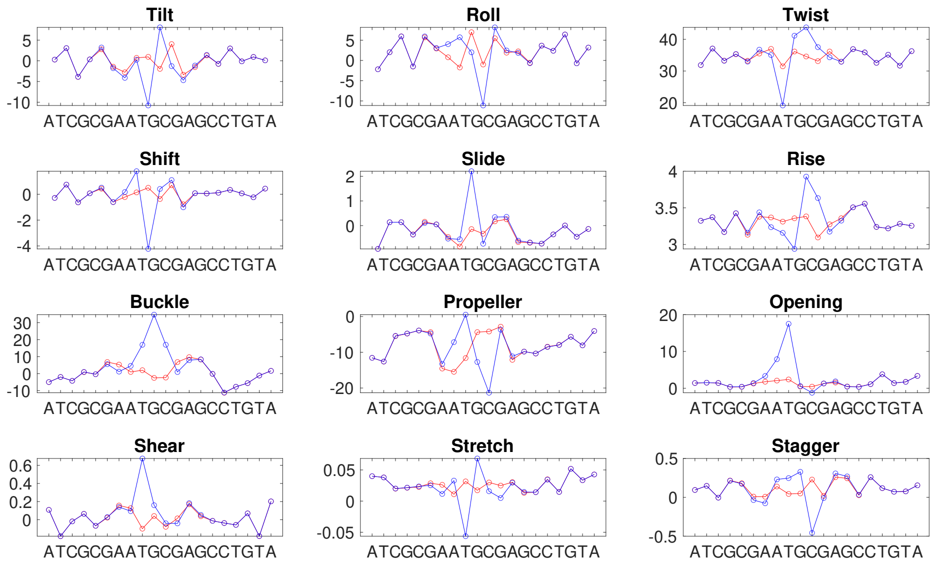

Figure 1: Helical parameters of the groundstate (red) and conditional groundstate (in blue) for the sequence S in Curves+ sense (translations in Angstroms and rotations in degrees). The rows 1 and 2 are the components of the inters while rows 3 and 4 are components of the intras. Rows 1 and 3 are the rotation parts while rows 2 and 4 are the translation parts. See Figure 1 of Serie 5 for the cartoon of the helical parameters.

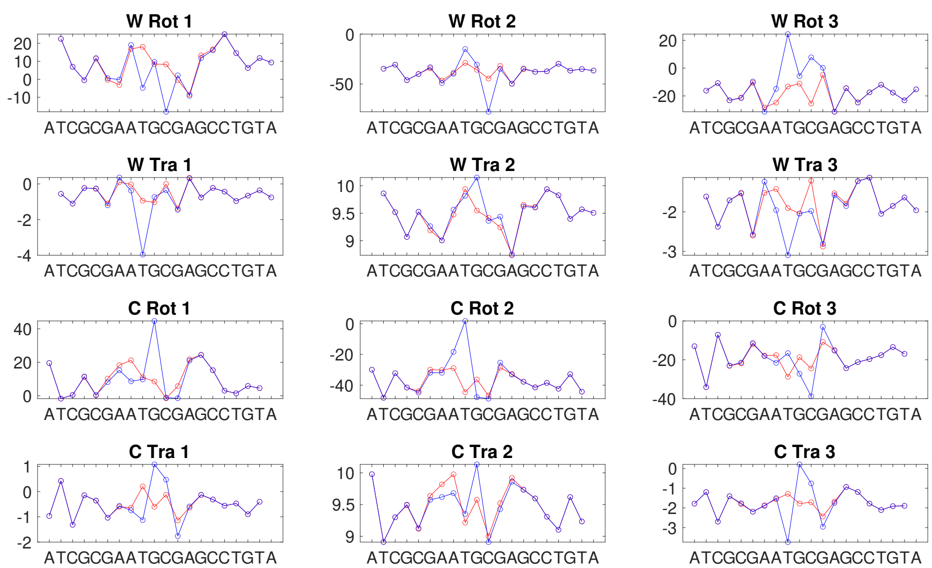

Figure 2: Phosphate coordinates of the groundstate (red) and conditional groundstate (in blue) for the sequence S (translations in Angstroms and rotations in degrees). The rows 1 and 2 correspond to Watson (W) phosphate while rows 3 and 4 correspond to Crick (C) phosphate. Rows 1 and 3 are the rotation parts while rows 2 and 4 are the translation parts. See Figure 2 Serie 5 for the cartoon of phosphates.

3 On the average of rotation matrices sharing a common (deterministic) axis

Let $\mathcal{Q} = \{Q_k\}_{k=1}^N \subset \mathrm{SO}(3)$ an ensemble of rotation matrices sharing a common unitary axis of rotation denoted by $\mathbf{u}$. The norm of the mean value is computed as the supremum of the vectorial norm $\|\frac{1}{N}\sum_{k=1}^N Q_k x\| = \|\frac{1}{N}\sum_{k=1}^N y_k\|$ where $y_k := Q_k x$ and $\|x\| = 1$. As x is a unit vector y_k is also unitary, by using the triangular inequality we obtain that

$$\left\|\frac{1}{N}\sum_{k=1}^{N} y_k\right\| \leq \frac{1}{N}\sum_{k=1}^{N}\|y_k\| = 1. \tag{6}$$

Let now $x = \mathbf{u}$, this implies that $y_k := Q_k u = u$ and thus the triangular inequality in the previous equation is actually an equality and the axis of rotation is the vector that satisfy the supremum, i.e., $\|\langle Q\rangle\| = \sup_{\|x\|=1}\|\langle Q\rangle x\| = \|\langle Q\rangle \mathbf{u}\| = 1$.

Assume now that at least one of the rotation matrix in $\mathcal{Q}$ is not a rotation matrix around the axis $\mathbf{u}$. This implies that for any choice of $x \in \mathbb{R}^3$ the vectors $y_k = Q_k x$ will not all be co-linear and thus $\|\langle Q\rangle\| < 1$. In other words, when at least one rotation matrix has a different rotation axis, for any choice of x the euclidean average of the unit vectors $y_k : Q_k x$ will be a point in the interior of the unit sphere.

4 On the parametrization of junction displacement using quaternions

1. Lets define $u = Cay(Q)$ the Cayley vector of $Q \in \mathrm{SO}(3)$ with $\|u\| = \tan\frac{\theta}{2}$, $0 \leq \theta < \pi$. We need to find $q \equiv q(u) \in \mathbb{R}^4$ such that $\|q\| = 1$ and q satisfy the relations (4) in the statement of this exercise. Thus, we have that

$$\begin{aligned}
\|(q_0, \mathbf{q})\| &= \sqrt{q_0^2 + \|\mathbf{q}\|^2} = \sqrt{\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}} = \cos\frac{\theta}{2}\sqrt{1 + \tan^2\frac{\theta}{2}} \\
&= \cos\frac{\theta}{2}\sqrt{1 + \|u\|^2} \\
&= \cos\frac{\theta}{2}\|(1, u)\|.
\end{aligned}$$

Finally we found that $q = \cos\frac{\theta}{2}(1, u) \in \mathbb{R}^4$ is a quaternion that satisfy $\|q\| = 1$ and the relations (4) in the statement of this exercise.

2. We recall that the Euler-Rodrigues formula reads:

$$Q(u) = \frac{1 - \|u\|^2}{1 + \|u\|^2}\mathrm{I} + \frac{2}{1 + \|u\|^2}[u\times] + \frac{2}{1 + \|u\|^2}u \otimes u, \tag{7}$$

see exercise 1.2 session 3 for details. We will use now the previous part and we will define $q = (q_0, \mathbf{q}) = (q_0, q_1, q_2, q_3) = (\cos\frac{\theta}{2}, \cos\frac{\theta}{2}u)$ where $\dfrac{\mathbf{q}}{\cos\frac{\theta}{2}} = u$. Then the following identities holds

$$
\begin{aligned}
\frac{1-\|u\|^2}{1+\|u\|^2} &= \cos^2\frac{\theta}{2}-\sin^2\frac{\theta}{2} = q_0^2-q_1^2-q_2^2-q_3^2,\\
\frac{2}{1+\|u\|^2}[u\times] &= 2q_0[\mathbf{q}\times] = \begin{bmatrix} 0 & -2q_0q_3 & 2q_0q_2\\ 2q_0q_3 & 0 & -2q_0q_1\\ -2q_0q_2 & 2q_0q_1 & 0\end{bmatrix},\\
\frac{2}{1+\|u\|^2}u\otimes u &= 2\mathbf{q}\otimes\mathbf{q} = \begin{bmatrix} q_1^2 & q_1q_2 & q_1q_3\\ q_1q_2 & q_2^2 & q_2q_3\\ q_1q_3 & q_2q_3 & q_3^2\end{bmatrix}.
\end{aligned}
$$

The result is obtained just by using the previous identities. Now after using the above equations in (7) one will get the desired expression of $Q(q)$.

3. We recall that in the cgDNA+ model we have a specific scaling for the rotations, thus one has to be careful when using, for example, the Euler-Rodrigues formula or the Cayley transform. In fact in the cgDNA+ model we use a scaling in such a way that if u is a Cayley vector, $\|u\| = 10\tan\frac{\theta}{2}$ (we have already done one exercise on scaling of Cayley i.e. Qu3 serie 6). For the purpose of this exercise, you have to set $U = u_2/10$ where u_2 is the Cayley vector related to the second inter rotational coordinates which is related to the rotation Q_2. In order to get the quaternions for the matrices R_2, R_3 first you have to use the inverse Cayley transform (defined in Qu 4 of session 5) with $M = R_2, R_3$ to get the Cayley vector ρ_2, ρ_3. Do not confuse with the notation, here ρ_2, ρ_3 represent the Cayley vector corresponding to R_2, R_3. Once you have the Cayley vectors ρ_2, ρ_3 and U then you can use the part-1 of this exercise to compute the quaternions q^{R_2}, q^{R_3}, and q^{Q_2}. Finally, compute the quaternion multiplication to verify that $q^{R_2}\circ q^{Q_2} = q^{R_3}$ and then use the part-2 to verify that $R_3 = R(q^{R_3})$.