

1 Palindromic symmetry of a shape vector and stiffness matrix

1. The shape vector and covariance matrix do not satisfy palindromic symmetry conditions: the biggest difference between the shape elements is 0.18 and, by coincidence, it's also 0.18 for the covariance.
2. By looking at the plot we can see, that most of differences between symmetrized and observed shape elements are actually quite small, under 0.03 in absolute value, and the biggest differences are at the ends of the molecule.
3. First compute $D = C + \bar{\mathbf{w}} \otimes \bar{\mathbf{w}}$ and then symmetrize it. We can see from the plots that the biggest differences are again towards the ends of the molecule.
4. In the following table we reported the result of the computations:

	KLD	stiffness part	mean part
$D(\rho_{obs}^{sym}(S), \rho_{obs}(S))$	0.3440	0.2724	0.0716
$D(\rho_{band}^{sym}(S), \rho_{obs}^{sym}(S))$	11.4417	11.4417	0
$D(\rho_{cgDNA}(S), \rho_{band}^{sym}(S))$	5.4556	3.4216	2.0340

2 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

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

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 1, Session 9, 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 1 of Session 9:

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

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 1 of Session 9 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 :

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

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

We obtain that

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

where $\bar{\mathbf{x}} = \hat{\mathbf{x}}_1 + \Sigma_{12} \Sigma_{22}^{-1} (\mathbf{a} - \hat{\mathbf{x}}_2)$, $\bar{\Sigma} = \Sigma_{11} - \Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}$.

3 On the computation of conditionals of the cgDNA probability distribution

1. Let us recall that we are working on the following Gaussian:

$$\rho(\mathbf{w}; S, \mathcal{P}) = \frac{1}{Z} \exp \left\{ -\frac{1}{2} \begin{bmatrix} w_1 - \hat{w}_1 \\ y_i - \hat{y}_i \\ w_2 - \hat{w}_2 \end{bmatrix} \begin{bmatrix} A & B & 0 \\ B^T & C & D^T \\ 0 & D & E \end{bmatrix} \begin{bmatrix} w_1 - \hat{w}_1 \\ y_i - \hat{y}_i \\ w_2 - \hat{w}_2 \end{bmatrix} \right\}. \quad (6)$$

We can now define the following matrices :

$$\begin{aligned} K_{11} &= \begin{bmatrix} A & 0 \\ 0 & E \end{bmatrix}, \\ K_{12} &= \begin{bmatrix} B \\ D \end{bmatrix}, \\ K_{22} &= C, \\ K &= \begin{bmatrix} K_{11} & K_{12} \\ K_{12}^T & K_{22} \end{bmatrix}, \end{aligned}$$

and the following vectors:

$$\begin{aligned} \mathbf{x}_1 &= \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \\ \mathbf{x}_2 &= y_i, \\ \mathbf{x} &= \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}. \end{aligned}$$

Finally we define $\hat{\mathbf{x}}$ as done for \mathbf{x} but for the corresponding "hat" variables. Finally, we have rearranged the stiffness matrix and the mean of (6) in such a way that we can reuse the decomposition obtained in the previous Exercise, Equation (2), in order to get the conditional distribution for the variable $\hat{\mathbf{x}}_1 = (w_1, w_2)$. Finally we obtain that

$$\begin{aligned} \bar{w}_1 &= \hat{w}_1 - A^{-1} B (\mathbf{a} - \hat{y}_i) \\ \bar{w}_2 &= \hat{w}_2 - E^{-1} D (\mathbf{a} - \hat{y}_i) \end{aligned}$$

where we fixed $y_i = \mathbf{a}$. You can now modify the code and run the computation for the given arguments.

4 Square roots in SE(3)

Using a direct computation one can easily find that

$$B = \begin{bmatrix} Q^{\frac{1}{2}} & (I + Q^{\frac{1}{2}})^{-1} q \\ 0_3^T & 1 \end{bmatrix} \quad (7)$$

Remark: Using the square root of a SE(3) element we can define the mid frames between two frames (R^n, r^n) and (R^{n+1}, r^{n+1}) , or more precisely the mid rigid body motion between rigid body n and rigid body $n + 1$. Let first define the rigid body configuration for the rigid body n as

$$g_n = \begin{bmatrix} R^n & r^n \\ 0_3^T & 1 \end{bmatrix}, \quad (8)$$

equivalently we can define the rigid body configuration for the rigid body $n + 1$.

The mid rigid body motion from n to $n + 1$ is then defined as:

$$g_{n+\frac{1}{2}} = g_n (g_n^{-1} g_{n+1})^{\frac{1}{2}}. \quad (9)$$

The rotation part of $g_{n+\frac{1}{2}}$ is $R_{n+\frac{1}{2}} = R_n (R_n^T R_{n+1})^{\frac{1}{2}}$ which correspond to the definition we used for the orientation of the mid frames, but the translational part $r_{n+\frac{1}{2}}$ is more complicated than the definition we used (mean value of the position r_n and r_{n+1}). One of the disadvantage of using (9) is that the mid rigid body motion from n to $n + 1$ is different (in the translation part) than the mid rigid body motion from $n + 1$ to n . This is not the case for the definition we adopted in the cgDNA model.

5 Statistical physics for ideal polymer chains (Optional)

1) The recurrence relation gives

$$r_n = r_0 + l \sum_{k=0}^{n-1} t_k,$$

which implies

i)

$$\langle (r_n - r_0) \cdot t_0 \rangle = l \sum_{k=0}^{n-1} \langle t_k \cdot t_0 \rangle = l \sum_{k=0}^{n-1} c_{k,0}$$

and

$$\langle \|r_n - r_0\|^2 \rangle = l^2 \sum_{k=0}^{n-1} \sum_{l=0}^{n-1} \langle t_k \cdot t_l \rangle = nl^2 + 2l^2 \sum_{k=0}^{n-1} \sum_{l=0}^{k-1} c_{k,l}.$$

ii) Consequently, using the previous expressions, we find

$$\langle (r_n - r_0) \cdot t_0 \rangle = l \sum_{k=0}^{n-1} \alpha^k = l \frac{1 - \alpha^n}{1 - \alpha}$$

and

$$\langle \|r_n - r_0\|^2 \rangle = nl^2 + 2l^2 \sum_{k=0}^{n-1} \sum_{l=0}^{k-1} \alpha^{k-l} = nl^2 + 2l^2 \left[n \frac{\alpha - \alpha^n}{1 - \alpha} - \alpha \frac{1 - \alpha^n}{1 - \alpha} + n^2 \frac{\alpha^n}{1 - \alpha} \right].$$

2) Observe that for all θ we can write

$$t_{n+1} \cdot t_n = \cos(\theta) = \cos(\hat{\theta}) \cos(\theta - \hat{\theta}) - \sin(\hat{\theta}) \sin(\theta - \hat{\theta}).$$

Using then the symmetry hypotheses on the probability distribution around $\hat{\theta}$ leads to

$$\langle t_{n+1} \cdot t_n \rangle = \cos(\hat{\theta}) \langle \cos(\theta - \hat{\theta}) \rangle$$

since the function $\sin(\theta - \hat{\theta})$ is odd.