1 Solving stationarity conditions for the cgDNA model with parameter continuation

Download here `http://lcvmwww.epfl.ch/teaching/modelling_dna/public_files/Lecture_Notes_cgDNAeq.pdf`.
In the lecture note for cgDNAeq we presented the following constrained minimization problem

$$\begin{cases} \min E(x) \text{ subject to} \\ (z_1, \dots, z_{N-1}) \in C, \end{cases} \tag{1}$$

where $E(x) = \frac{1}{2}(x - \hat{x}) \cdot K(x - \hat{x})$ is the cgDNA energy, $x = (y_1, z_1, \dots, z_{N-1}, y_N) \in \mathbb{R}^{12N-6}$ are the cgDNA coordinates, $y_n \in \mathbb{R}^6$ denote the intras variables, $z_n = (u_n, v_n) \in \mathbb{R}^6$ denote the inter variables, and C is the following constraint set

$$C = \{(z_1, \dots, z_{N-1}) | \Phi(z_1, \dots, z_{N-1}) = \mathbf{g}^*\}, \tag{2}$$

with

$$\Phi(z_1, \dots, z_{N-1}) = \prod_{n=1}^{N-1} a(z_n) = \prod_{n=1}^{N-1} \begin{bmatrix} Q(u_n) & Q(u_n)^{\frac{1}{2}} v_n \\ 0 & 1 \end{bmatrix}. \tag{3}$$

The constraint set C requires that the rigid body motion from the first to the last base pair is prescribed to take a value $\mathbf{g}^* \in SE(3)$,

$$\mathbf{g}^* = \begin{bmatrix} \mathbf{R}^* & \mathbf{r}^* \\ 0 & 1 \end{bmatrix}. \tag{4}$$

Without loss of generality the first base pair is chosen to be the identity matrix I_4. Then, as we prescribed in the notes for cgDNAeq, the first–order stationarity condition of the problem (1) is

$$K(x - \hat{x}) - \begin{bmatrix} 0 \\ L_{z_1}^T \mathrm{Ad}_I^T \boldsymbol{\lambda} \\ 0 \\ \dots \\ L_{z_{N-1}}^T \mathrm{Ad}_{\mathbf{g}_{N-1}}^T \boldsymbol{\lambda} \\ 0 \end{bmatrix} = 0, \tag{5}$$

$$\prod_{n=1}^{N-1} a(z_n) - \mathbf{g}^* = 0, \tag{6}$$

You can download from `http://lcvmwww.epfl.ch/teaching/modelling_dna/public_files/cgDNAeq_code.zip` a set of (rudimentary) MATLAB scripts implementing a Newton solve finding of solutions of the stationarity conditions (5) with the boundary condition (6). Check that the scripts `cgDNAeq` and `evalStatCond` actually implements the solution of the system (5-6).

Parameter Continuation with cgDNAeq

The goal of parameter continuation methods is to study solutions of parameter dependent nonlinear systems of the form

$$F(\omega;\epsilon) = 0 \in \mathbb{R}^N,\ \ \omega \in \mathbb{R}^N, \epsilon \in \mathbb{R}, \tag{7}$$

as the parameter ϵ varies. In this exercise we want to apply the parameter continuation method to the stationarity condition (5-6) where the parameter continuation varying the third component of $\mathbf{r}^*$ in the boundary condition $\mathbf{g}^*$. More precisely we want to study solutions of the following problem

$$F(\omega;\mathbf{g}^* + \epsilon d\mathbf{g}) = 0 \in \mathbb{R}^{12N}, \tag{8}$$

where $\omega = (x, \boldsymbol{\lambda}) \in \mathbb{R}^{12N}$, $d\mathbf{g} \in \mathbb{R}^{4\times4}$ has all zero entries except for the (3,4) position, and ϵ is a given real value, i.e,

$$\mathbf{g}^* + \epsilon d\mathbf{g} = \begin{bmatrix} \mathbf{R}^* & \mathbf{r}^* + \epsilon d\mathbf{r} \\ 0 & 1 \end{bmatrix}, d\mathbf{r} = \begin{bmatrix} 0 \\ 0 \\ dr_z \end{bmatrix} \tag{9}$$

For small value of ϵ one can numerically solve the problem (8) once the solution for $\epsilon = 0$ is known.

Write a MATLAB script that solve the following family of problems:

$$F(\omega;\mathbf{g}^* + \epsilon_n d\mathbf{g}) = 0, \forall \epsilon_n \in \mathbb{Z}, \tag{10}$$

where $\omega = (x, \boldsymbol{\lambda}) \in \mathbb{R}^{12N}$, and the non zero entry of $d\mathbf{g}$, denoted by dr_z, is a fixed real value. Test your script on the two DNA sequences downloaded with cgDNAeq, poly$(AT)_{79}$ and CAP, by performing pulling and pushing numerical experiments. The output of the computations we are interested in are:

i) The moments and the forces as a function of ϵ_n,

ii) The 3D reconstruction of the shapes as function of ϵ_n.

Produce the above plots for the two given sequences.
[Note on the units of lambda: The three first components of lambda correspond to the moments, while the last three components correspond to the forces. The moments come in the units of pico Newton Angstroms per k_BT ($pN\text{Å}(k_BT)^{-1}$), while the forces come in pico Newton per k_BT ($pN(k_BT)^{-1}$). For the plots multiply all the components of lambda by 42 in order to obtain the units $pN\text{Å}$ for the moments and pN for the forces.]