Mathematical Modelling of DNA
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SESSION 12: SOLUTIONS A. PATELLI

1 Principle of maximum entropy parameter estimation for banded stiffness matrices

According to the maximum entropy principle, the distribution $\rho_{ME}(x)$ can be defined as

$$\rho_{ME} = \text{argmin}_{\rho \in C} S[\rho] \text{ where } S[\rho] = \int_{\Omega} \rho(x) \ln \rho(x) dx.$$

The Lagrange multiplier method allows to write the distribution $\rho_{ME}(x) \in C$ as the solution of

$$\int_{\Omega} \{(1 + \ln \rho_{ME}(x)) - \lambda_0 - \lambda_1 \cdot x - [[\lambda_2]] : (x \otimes x)\} \delta\rho(x) dx = 0 \quad (*)$$

for any $\delta\rho \in \mathrm{L}^1(\Omega)$ and for some Lagrange multipliers $\lambda_0 \in \mathbb{R}$, $\lambda_1 \in \mathbb{R}^{12n-6}$ and $\lambda_2 \in \mathbb{R}^{(12n-6)\times(12n-6)}$. Note that we have used that the first variation of the functional $S[\rho]$ can be written as

$$\delta S[\rho]\delta\rho = \int_{\Omega} (1 + \ln \rho(x))\delta\rho(x) dx$$

for any $\rho, \delta\rho \in \mathrm{L}^1(\Omega)$ and that

$$\delta \left\{ \int_{\Omega} \phi(x)\rho(x) dx \right\} \delta\rho = \int_{\Omega} \phi(x)\delta\rho(x) dx$$

for any $\phi \in \mathrm{L}^1(\Omega)$ to deduce $(*)$. A sufficient condition is then that the distribution $\rho_{ME}(x)$ is normal, i.e. that it is of the form

$$\rho_{ME}(x) = \frac{1}{Z} \exp \left\{ -\frac{1}{2}(x - a) \cdot A(x - a) \right\}$$

with

$$(\lambda_0 - 1) + \lambda_1 \cdot x + [[\lambda_2]] : (x \otimes x) = -\frac{1}{2}(x - a) \cdot A(x - a) - \ln Z \quad (**)$$

for all $x \in \Omega$. Moreover, since we have the constraints $\rho_{ME}(x) \in C$, we can directly deduce that we have to define

$$a = \mu, A = K_{ME} \text{ and } Z = \sqrt{\det(2\pi K_{ME})}$$

according the identities regarding the first and second moment of a normal distribution. We note that the equality $(**)$ allows then to compute explicitly the values of the Lagrange multipliers λ_0, λ_1 and λ_2.

2 Estimate of mean and stiffness from MD simulation data

1. One can observe that the raw stiffness matrix has the most of the non zero entries near the diagonal, in fact by using `plot2Dmatrix` one can observe that the most of the non zero entries are in the stencil. On the contrary the raw covariance matrix is dense and do not present any specific pattern around the diagonal.

2. In order to get the right scaling you should multiply the rotation-rotation blocks by 25, the rotation-translation block by 5 and the translation-translation by 1.

3 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