DNA Modelling Course
Exercise Session 1
Summer 2006 Part I

1 The length scales of DNA

Every diploid human cell[1], in the non-dividing state, contains twice the human genome ($\simeq 3 \cdot 10^9$ base-pairs of DNA) for a total of about $6 \cdot 10^9$ base-pairs of DNA. The diameter of a typical human nucleus cell is of the order of $10\mu\text{m} = 10^5$Å, where

$$\mu\text{m} = 10^{-6}\text{m}, \quad \text{nm} = 10^{-9}\text{m}, \quad \text{Å} = 10^{-10}\text{m}.$$

(a) By treating the DNA as a cylinder of length 3.4Å per base-pair, calculate the total length of DNA in any cell. Compare this to the diameter of the cell.

(b) By treating the DNA as a cylinder of diameter 20Å, calculate the total volume of DNA in any cell. Compare this to the total volume of the cell, if it is assumed to be spherical.

(This exercise was taken from the book 'Understanding DNA', C.R. Callandine, H.R. Drew which is listed on the Reading List of the DNA course Home page, see http://lcvmwww.epfl.ch)

2 Rotations in three dimensions

Consider any matrix $\boldsymbol{Q} \in \mathbb{R}^{3\times3}$, i.e., $\boldsymbol{Q}$ is a 3×3 matrix with real entries, such that $\boldsymbol{Q}^{-1} = \boldsymbol{Q}^T$ and $\det[\boldsymbol{Q}] = 1$. The matrix $\boldsymbol{Q}$ is called a *proper rotation* because if $\{\boldsymbol{v}_i\}$ is any right-handed, orthonormal basis for $\mathbb{R}^3$, then so too is $\{\boldsymbol{Q}\boldsymbol{v}_i\}$.

(a) Show that all the eigenvalues of $\boldsymbol{Q}$ are on the unit circle in the complex plane. Hint: For this part and the next it is helpful to know the identity

[1] A diploid cell contains two copies of each chromosome, plus a couple X X for women and a couple X Y for men.

$\boldsymbol{Mx} \cdot \boldsymbol{y} = \boldsymbol{x} \cdot \boldsymbol{M}^T \boldsymbol{y}$, and properties of the roots of polynomials with real coefficients. Moreover, it will be useful to express the determinant in terms of the eigenvalues.

(b) Show that $\boldsymbol{Q}$ always has an eigenvalue of unity, and so there is a unit vector $\boldsymbol{w}$ such that $\boldsymbol{Qw} = \boldsymbol{w}$. This vector defines the *axis of rotation* of $\boldsymbol{Q}$, and is in fact parallel to the axial vector[2] of the skew matrix $(\boldsymbol{Q} - \boldsymbol{Q}^T)$. Can a proper rotation have more than one axis?

(c) Let $\boldsymbol{v}$ be any unit vector orthogonal to $\boldsymbol{w}$. Show that $\boldsymbol{Qv}$ is also a unit vector orthogonal to $\boldsymbol{w}$ and that the angle $0 \le \theta < 2\pi$ (measured counter-clockwise about $\boldsymbol{w}$) between $\boldsymbol{v}$ and $\boldsymbol{Qv}$ satisfies the relation

$$1 + 2\cos\theta = \mathrm{tr}(\boldsymbol{Q}), \tag{2.1}$$

where the trace of a matrix is defined as the sum of its diagonal entries, that is,

$$\mathrm{tr}(A) = \sum_{i=1}^{n} a_{ii}, \qquad \text{for } A = (a_{ij})_{i,j \in R^n}.$$

The angle θ defines the *rotation angle* associated with $\boldsymbol{Q}$. The effect of $\boldsymbol{Q}$ on *any* vector is to rotate it about the direction $\boldsymbol{w}$ by the angle θ. (For this part it is helpful to express $\boldsymbol{Q}$ in the basis $\{\boldsymbol{w}, \boldsymbol{v}, \boldsymbol{w} \times \boldsymbol{v}\}$.) Hint for showing (2.1): Express the trace $\mathrm{tr}(A)$ of a matrix A in terms of the eigenvalues!

3 Quaternion parametrization

There are many ways to characterize a general proper rotation matrix $\boldsymbol{Q} \in \mathbb{R}^{3\times 3}$ using only three or four parameters. But there is a theorem that there is no singularity-free three parameter description. Here we study a four-dimensional parametrization in terms of quaternions, which can be compared with the more standard Euler Angles description (see next page)[3].

[2] Recall that a skew matrix $W \in \mathbb{R}^{3\times 3}$ has a unique axial vector $w = (w_1, w_2, w_3)^T \in \mathbb{R}^3$ satisfying $Wv = w \times v$ for all $v \in \mathbb{R}^3$, that is,

$$W = \begin{pmatrix} 0 & -w_3 & w_2 \\ w_3 & 0 & -w_1 \\ -w_2 & w_1 & 0 \end{pmatrix}.$$

[3] This page was taken from the book 'Classical Mechanics', H.Goldstein.

By a *quaternion* we just mean an element $\boldsymbol{q} \in \mathbb{R}^4$ satisfying the condition

$$\boldsymbol{q} \cdot \boldsymbol{q} = q_1^2 + q_2^2 + q_3^2 + q_4^2 = 1.$$

To any quaternion $\boldsymbol{q}$ we associate a unique proper rotation $\boldsymbol{Q}$ according to the expression

$$\boldsymbol{Q}(\boldsymbol{q}) = \begin{pmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 & 2(q_1q_2 - q_3q_4) & 2(q_1q_3 + q_2q_4) \\ 2(q_1q_2 + q_3q_4) & -q_1^2 + q_2^2 - q_3^2 + q_4^2 & 2(-q_1q_4 + q_2q_3) \\ 2(q_1q_3 - q_2q_4) & 2(q_1q_4 + q_2q_3) & -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{pmatrix}.$$

If we denote the columns of $\boldsymbol{Q}(\boldsymbol{q})$ by $\boldsymbol{d}_i(\boldsymbol{q})$ $(i = 1, 2, 3)$, then the set $\{\boldsymbol{d}_i(\boldsymbol{q})\}$ is an oriented, orthonormal basis for $\mathbb{R}^3$, parameterized by $\boldsymbol{q}$.

(a) Let $\boldsymbol{q}$ be a quaternion, $\boldsymbol{Q}$ the associated rotation matrix as defined above and consider the vector $\boldsymbol{k} = (q_1, q_2, q_3)^T$. Assuming $\boldsymbol{k} \neq \boldsymbol{0}$, show that $\boldsymbol{k}$ defines the axis of rotation of $\boldsymbol{Q}$ in the sense that $\boldsymbol{Qk} = \boldsymbol{k}$. What can be said about $\boldsymbol{Q}$ if $\boldsymbol{k} = \boldsymbol{0}$?

(b) Show that q_4 defines the rotation angle θ associated with $\boldsymbol{Q}$ and $\boldsymbol{k} \neq \boldsymbol{0}$, namely, $\cos(\theta/2) = q_4$

(c) Given any quaternion $\boldsymbol{q}$, show that the set $\{\boldsymbol{q}, \boldsymbol{B}_1\boldsymbol{q}, \boldsymbol{B}_2\boldsymbol{q}, \boldsymbol{B}_3\boldsymbol{q}\}$ is an orthonormal basis for $\mathbb{R}^4$, where the matrices $\boldsymbol{B}_i \in \mathbb{R}^{4\times 4}$ $(i = 1, 2, 3)$ are defined by

$$\boldsymbol{B}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{3.1}$$

$$\boldsymbol{B}_2 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \tag{3.2}$$

and

$$\boldsymbol{B}_3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{3.3}$$