DNA Modelling Course Exercise Session 2 Winter 2003/04

SOLUTIONS

Kinematics of orthonormal frames and compo-1 nents of vectors I

(a) It is sufficient to prove (1.1) since (1.2) is shown in an analogous way. We consider the matrix $\boldsymbol{Q}(s,t) = [\boldsymbol{d}_1(s,t), \boldsymbol{d}_2(s,t), \boldsymbol{d}_3(s,t)], \boldsymbol{d}_i \in \mathbb{R}^3$ and define Q' to be the derivative wrt. s, that is¹,

$$oldsymbol{Q}' = \left[rac{\partial oldsymbol{d}_1}{\partial s}, rac{\partial oldsymbol{d}_2}{\partial s}, rac{\partial oldsymbol{d}_3}{\partial s}
ight]$$

First, we derive an expression for Q' which allows us to conlude Q' =SQ with S being skew-symmetric: As Q is a proper rotation matrix, we have $\mathbf{Q}' = \mathbf{Q}'(\mathbf{Q}^T \mathbf{Q}) = (\mathbf{Q}' \mathbf{Q}^T) \mathbf{Q}$. Thus, we only have to show that $\mathbf{S} := \mathbf{Q}' \mathbf{Q}^T$ is skew symmetric. But this follows from $(\mathbf{Q}')^T = (\mathbf{Q}^T)'$ and

$$\boldsymbol{Q}\boldsymbol{Q}^T = \mathrm{Id} \implies \boldsymbol{Q}'\boldsymbol{Q}^T + \boldsymbol{Q}(\boldsymbol{Q}^T)' = 0.$$

Conclusively, we obtain

$$\boldsymbol{Q}' = \boldsymbol{S}\boldsymbol{Q} = [\boldsymbol{S}\boldsymbol{d}_1, \boldsymbol{S}\boldsymbol{d}_2, \boldsymbol{S}\boldsymbol{d}_3] \tag{1.1}$$

with $S = Q'Q^T$ being a skew symmetric matrix.

Therefore, it exists a *unique* axial vector² \boldsymbol{u} such that $\boldsymbol{S}\boldsymbol{z} = \boldsymbol{u} \times \boldsymbol{z}$ for all z, that is, using the notation from Session 1 (solution!) $S = u^{\times}$. Hence, equation (1.1) is expressed

$$Q' = u^{\times}Q,$$

which is, by definition,

$$\frac{\partial d_i}{\partial s} = u \times d_i, \qquad i = 1, 2, 3.$$

¹The derivative of a matrix is the matrix of the derivatives of its components.

²Compare Exercise 2 of Session 1!!

Note, that the existence of a second vector v with $Q' = v^{\times}Q$ would immediately imply $S = v^{\times}$ resulting in v = u!

(b) It is sufficient to prove (1.6) and (1.7). The results for t can then be derived analogously! In the following we make use of

$$d_i = \varepsilon_{ijk} d_j \times d_k, \quad \text{for fixed } i, j, k \text{ with } i \neq j \neq k \qquad (1.2)$$

$$d_i = \sum_{k,j} \frac{1}{2} \varepsilon_{ijk} d_j \times d_k.$$
(1.3)

Note that both representations of d_i are valid, where (1.3) obviously follows from (1.2) (but not vice versa). In the same way we could immediately infer from (1.6) to (1.7). (1.2) is used to show (1.6), whereas we prefer equality (1.3) in order to show (1.7). We moreover need the following rule for the vector product:

$$(\boldsymbol{v} \times \boldsymbol{w}) \cdot \boldsymbol{z} = (\boldsymbol{w} \times \boldsymbol{z}) \cdot \boldsymbol{v} = (\boldsymbol{z} \times \boldsymbol{v}) \cdot \boldsymbol{w}.$$

Now, we obtain from (1.2) for fixed i, j, k and $i \neq j \neq k$

$$u_i = u \cdot d_i = \varepsilon_{ijk} u \cdot (d_j \times d_k) = \varepsilon_{ijk} (d_j \times d_k) \cdot u$$
$$= \varepsilon_{ijk} (u \times d_j) \cdot d_k = \varepsilon_{ijk} \frac{\partial d_j}{\partial s} \cdot d_k.$$

Note that we deal with real vectors here, such that $\boldsymbol{v} \cdot \boldsymbol{z} = \boldsymbol{z} \cdot \boldsymbol{v}$. In order to verify (1.7) we use (1.3) instead of (1.2) and exploit bilinearity of the scalar product for real vectors:

$$\begin{split} u_i &= u \cdot d_i = \frac{1}{2} \sum_{j,k} \varepsilon_{ijk} u \cdot (d_j \times d_k) = \frac{1}{2} \sum_{j,k} \varepsilon_{ijk} (d_j \times d_k) \cdot u \\ &= \frac{1}{2} \sum_{j,k} \varepsilon_{ijk} (u \times d_j) \cdot d_k = \frac{1}{2} \sum_{j,k} \varepsilon_{ijk} \frac{\partial d_j}{\partial s} \cdot d_k. \end{split}$$

(c) Note that we now have

$$\frac{\partial}{\partial s}(\boldsymbol{d}_i(\boldsymbol{q}(s))) = \boldsymbol{u}(s) \times \boldsymbol{d}_i(\boldsymbol{q}(s)), \qquad i = 1, 2, 3.$$

Using the hints, we obtain for fixed i, j, k such that ijk is a cyclic permutation of 123:

$$u_i = u \cdot d_i(q) = u \cdot (d_j \times d_k) = (u \times d_j) \cdot d_k = \frac{\partial}{\partial s} (d_j(q(s))) \cdot d_k$$
$$= \left(\frac{\partial d_j}{\partial q}(q(s))\right) \frac{\partial q}{\partial s} \cdot d_k = \frac{\partial q}{\partial s} \cdot (D_j(q(s))) d_k = 2 \frac{\partial q}{\partial s} \cdot B_i q.$$

The result for t is derived analogously.

2 Kinematics II

(a) We remark that for any two vectors $\boldsymbol{a}(s), \boldsymbol{b}(s) \in \mathbb{C}^3$ we have

$$rac{\partial}{\partial s}(oldsymbol{a}\cdotoldsymbol{b}) = rac{\partial oldsymbol{a}}{\partial s}\cdotoldsymbol{b} + oldsymbol{a}\cdotrac{\partial oldsymbol{b}}{\partial s}, \ rac{\partial}{\partial s}(oldsymbol{a} imesoldsymbol{b}) = rac{\partial oldsymbol{a}}{\partial s} imesoldsymbol{b} + oldsymbol{a} imesrac{\partial oldsymbol{b}}{\partial s},$$

which follows easily from the product rule, the fact that the derivative of the vectors is defined componentwise and the definition of inner product and vector product, respectively. Taking the derivative we have

$$\frac{\partial}{\partial s}(\boldsymbol{y} \cdot \boldsymbol{e}_i) = \frac{\partial \boldsymbol{y}}{\partial s} \cdot \boldsymbol{e}_i + \boldsymbol{y} \cdot \frac{\partial \boldsymbol{e}_i}{\partial s} = \frac{\partial \boldsymbol{y}}{\partial s} \cdot \boldsymbol{e}_i$$

The last equation holds since $\{e_1, e_2, e_3\}$ is a fixed basis. Using the variable frame d_i we get

$$\begin{array}{ll} \displaystyle \frac{\partial \boldsymbol{y}}{\partial s} &=& \displaystyle \frac{\partial}{\partial s}(y_i\boldsymbol{d}_i) = \frac{\partial y_i}{\partial s}\boldsymbol{d}_i + y_i\frac{\partial \boldsymbol{d}_i}{\partial s} = & \displaystyle \frac{\partial y_i}{\partial s}\boldsymbol{d}_i + y_i(\boldsymbol{u}\times\boldsymbol{d}_i) \\ &=& \displaystyle \frac{\partial y_i}{\partial s}\boldsymbol{d}_i + (\boldsymbol{u}\times y_i\boldsymbol{d}_i) = & \displaystyle \frac{\partial y_i}{\partial s}\boldsymbol{d}_i + \boldsymbol{u}\times\boldsymbol{y}, \end{array}$$

and therefore

$$\frac{\partial \boldsymbol{y}}{\partial s} \cdot \boldsymbol{d}_i = \frac{\partial y_i}{\partial s} + (\boldsymbol{u} \times \boldsymbol{y}) \cdot \boldsymbol{d}_i.$$
(2.1)

The results for t can be derived analogously.

- (b) Simply set y = u in (2.1) and use $u \times u = 0$. Analogously for t.
- (c) We have

$$\frac{\partial^2 \boldsymbol{d}_i}{\partial s \partial t} = \frac{\partial}{\partial s} (\omega \times \boldsymbol{d}_i) = \frac{\partial \omega}{\partial s} \times \boldsymbol{d}_i + \omega \times (\boldsymbol{u} \times \boldsymbol{d}_i)$$
(2.2)

$$\frac{\partial^2 \boldsymbol{d}_i}{\partial t \partial s} = \frac{\partial}{\partial t} (\boldsymbol{u} \times \boldsymbol{d}_i) = \frac{\partial \boldsymbol{u}}{\partial s} \times \boldsymbol{d}_i + \boldsymbol{u} \times (\boldsymbol{\omega} \times \boldsymbol{d}_i)$$
(2.3)

Using smoothness of the d_i we have $\frac{\partial^2 d_i}{\partial t \partial s} = \frac{\partial^2 d_i}{\partial s \partial t}$ and therefore

$$\frac{\partial \omega}{\partial s} \times \boldsymbol{d}_i - \frac{\partial \boldsymbol{u}}{\partial t} \times \boldsymbol{d}_i = \boldsymbol{u} \times (\omega \times \boldsymbol{d}_i) - \omega \times (\boldsymbol{u} \times \boldsymbol{d}_i) \qquad (2.4)$$

Using now the relations

$$(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{c} = (\boldsymbol{a} \cdot \boldsymbol{c}) \boldsymbol{b} - (\boldsymbol{b} \cdot \boldsymbol{c}) \boldsymbol{a}$$
$$\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c}) = (\boldsymbol{c} \cdot \boldsymbol{a}) \boldsymbol{b} - (\boldsymbol{b} \cdot \boldsymbol{a}) \boldsymbol{c}$$
(2.5)

where a, b, c are three arbitrary vectors, we get from (2.4)

$$\left[\frac{\partial \omega}{\partial s} - \frac{\partial \boldsymbol{u}}{\partial t}\right] \times \boldsymbol{d}_i = (\boldsymbol{u} \cdot \boldsymbol{d}_i)\omega - (\omega \cdot \boldsymbol{d}_i)\boldsymbol{u} = (\boldsymbol{u} \times \omega) \times \boldsymbol{d}_i \qquad (2.6)$$

which concludes the proof.