DNA Modelling Course
Exercise Session 2
Summer 2006 Part I

1 Kinematics of orthonormal frames and components of vectors I

Throughout the course we will make use of components of vectors in a non-fixed reference frame. These exercises introduce the necessary kinematics (i.e. geometry).
It is a general result that the columns $\{\boldsymbol{d}_i\}$ of a rotation matrix $\boldsymbol{Q}$ define an oriented, orthonormal basis for $I\!R^3$ and vice-versa.
Furthermore if $\{\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3\}$ is right handed, i.e. $\boldsymbol{d}_3 = \boldsymbol{d}_1 \times \boldsymbol{d}_2$ then $\boldsymbol{Q}$ is a proper rotation matrix, i.e. $\det \boldsymbol{Q} = |Q| = 1$. In Session 1 we have directly seen this in the quaternion parametrization. We now consider families of proper rotation matrices parametrized by $s \in [a, b]$ and $t \geq 0$, and define $\{\boldsymbol{d}_1(s,t), \boldsymbol{d}_2(s,t), \boldsymbol{d}_3(s,t)\}$ to be an orthonormal frame so that the matrix $\boldsymbol{Q}(s,t)$ which has $\{\boldsymbol{d}_i(s,t)\}$ as its columns is our rotation matrix, i.e., $\boldsymbol{Q}\boldsymbol{Q}^T = \mathrm{Id} \quad \forall s, t$. We recall here that by orthonormal we mean $\boldsymbol{d}_i \cdot \boldsymbol{d}_j = \delta_{ij} \quad \forall s, t$ and that the following notations hold

- Kronecker delta
$$\delta_{ij} = \begin{cases} 1 & i = j, \\ 0 & else. \end{cases}$$

- Total antisymmetric tensor
$$\epsilon_{ijk} = \begin{cases} 1 & ijk = \text{cyclic permutation of } 123, \\ -1 & ijk = \text{cyclic permutation of } 132, \\ 0 & else. \end{cases}$$

- Vector product
$$(\boldsymbol{a} \times \boldsymbol{b})_i = \epsilon_{ijk} a_j b_k$$

The summation convention means to sum over repeated indices. Here are some examples :

$$\begin{aligned}
u_i d_i &\quad \text{means} \quad \sum_{i=1}^{3} u_i d_i \\
\varepsilon_{ijk} a_{im} &\quad \text{means} \quad \sum_{i=1}^{3} \varepsilon_{ijk} a_{im} \\
\varepsilon_{ijk} a_{ij} &\quad \text{means} \quad \sum_{i=1}^{3} \sum_{j=1}^{3} \varepsilon_{ijk} a_{ij} \\
\varepsilon_{ijk} a_{mn} &\quad \text{means} \quad \varepsilon_{ijk} a_{mn}
\end{aligned}$$

Important note: we will use the summation convention on repeated indices unless otherwise is stated.
Finally, whenever we use Roman font indices, e.g., i or j, we mean that they run through the values 1,2 and 3, that is, $i = 1, 2, 3$ for example.

(a) Assuming differentiability, show that there exists a single vector function $\boldsymbol{u} : [a, b] \times [0, \infty) \to \mathbb{R}^3$ and a single vector function $\omega : [a, b] \times [0, \infty) \to \mathbb{R}^3$ such that

$$\frac{\partial \boldsymbol{d}_i}{\partial s} = \boldsymbol{u} \times \boldsymbol{d}_i \qquad (i = 1, 2, 3), \tag{1.1}$$

$$\frac{\partial \boldsymbol{d}_i}{\partial t} = \omega \times \boldsymbol{d}_i \qquad (i = 1, 2, 3), \tag{1.2}$$

for all $s \in [a, b]$, $\forall t \geq 0$. As has been discussed in class, the vector ω is the angular velocity (in time) whereas $\boldsymbol{u}$ is called the Darboux vector (and can be considered as the 'angular velocity' in arc length).

(b) With the notation

$$u_i = \boldsymbol{u} \cdot \boldsymbol{d}_i \tag{1.3}$$

$$\omega_i = \omega \cdot \boldsymbol{d}_i \tag{1.4}$$

so that

$$\begin{aligned}
\boldsymbol{u} &= u_i \boldsymbol{d}_i \\
\omega &= \omega_i \boldsymbol{d}_i \qquad (1.5)
\end{aligned}$$

show that the components u_i and ω_i in the director frame $\{\boldsymbol{d}_i\}$ are:

$$\begin{aligned} u_i &= \epsilon_{ijk} \frac{\partial \boldsymbol{d}_j}{\partial s} \cdot \boldsymbol{d}_k \\ \omega_i &= \epsilon_{ijk} \frac{\partial \boldsymbol{d}_j}{\partial t} \cdot \boldsymbol{d}_k \end{aligned} \tag{1.6}$$

with no summation over indices (that is for all $i \neq j \neq k$), or

$$\begin{aligned} u_i &= \frac{1}{2} \epsilon_{ijk} \frac{\partial \boldsymbol{d}_j}{\partial s} \cdot \boldsymbol{d}_k \\ \omega_i &= \frac{1}{2} \epsilon_{ijk} \frac{\partial \boldsymbol{d}_j}{\partial t} \cdot \boldsymbol{d}_k \end{aligned} \tag{1.7}$$

with summation over indices.

(c) In the quaternion parametrization, $\{\boldsymbol{d}_i(q)\}$ described in Session 1, show that

$$\begin{aligned} u_i(s) &= 2 \frac{\partial \boldsymbol{q}}{\partial s} \cdot \boldsymbol{B}_i \boldsymbol{q} \\ \omega_i(s) &= 2 \frac{\partial \boldsymbol{q}}{\partial t} \cdot \boldsymbol{B}_i \boldsymbol{q} \end{aligned} \tag{1.8}$$

Hint: Use the chain rule to compute the derivatives

$$\frac{\partial \boldsymbol{d}_j}{\partial s} = \frac{\partial \boldsymbol{d}_j}{\partial \boldsymbol{q}} \frac{\partial \boldsymbol{q}}{\partial s}$$

and note the following algebra

$$\boldsymbol{B}_1 \boldsymbol{q} = \frac{1}{2} \boldsymbol{D}_2(\boldsymbol{q}) \boldsymbol{d}_3(\boldsymbol{q})$$

$$\boldsymbol{B}_2 \boldsymbol{q} = \frac{1}{2} \boldsymbol{D}_3(\boldsymbol{q}) \boldsymbol{d}_1(\boldsymbol{q})$$

$$\boldsymbol{B}_3 \boldsymbol{q} = \frac{1}{2} \boldsymbol{D}_1(\boldsymbol{q}) \boldsymbol{d}_2(\boldsymbol{q})$$

where the $\boldsymbol{B}_i$ matrices were defined in session 1, and the three 4×3 matrices $\boldsymbol{D}_i(\boldsymbol{q})$ are defined by $\boldsymbol{D}_i(\boldsymbol{q}) = \left(\frac{\partial d_i}{\partial q}(\boldsymbol{q}) \right)^T$.

2 Kinematics of orthonormal frames and components of vectors II

(a) Let $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ be a fixed basis for $I\!R^3$ and $\boldsymbol{y}(s,t)$ be an arbitrary vector field with components $Y_i(s,t)$ with respect to $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ and $y_i(s,t)$ with respect to the orthonormal frame $\{\boldsymbol{d}_1(s,t)\boldsymbol{d}_2(s,t), \boldsymbol{d}_3(s,t)\}$, $s \in [a,b]$, $t \geq 0$.

Show that

$$\frac{\partial \boldsymbol{y}}{\partial s} \cdot \boldsymbol{e}_i = \frac{\partial Y_i}{\partial s} \qquad (i = 1,2,3), \tag{2.1}$$

$$\frac{\partial \boldsymbol{y}}{\partial t} \cdot \boldsymbol{e}_i = \frac{\partial Y_i}{\partial t} \qquad (i = 1,2,3). \tag{2.2}$$

for all $s \in [a,b]$, $\forall t \geq 0$. That is the $\boldsymbol{e}_i$ component of the derivative is just the derivative of the $\boldsymbol{e}_i$ component.

For the variable basis $\{\boldsymbol{d}_i(s,t)\}$ this result is not true for a general vector. Consider the relation between components of the derivative $\frac{\partial \boldsymbol{y}}{\partial s}$ w.r.t. $\{\boldsymbol{d}_i(s,t)\}$ and the derivative of the components $y_i(s,t)$.

Show that

$$\frac{\partial \boldsymbol{y}}{\partial s} \cdot \boldsymbol{d}_i = \frac{\partial y_i}{\partial s} + (\boldsymbol{u} \times \boldsymbol{y}) \cdot \boldsymbol{d}_i \qquad (i = 1,2,3), \tag{2.3}$$

$$\frac{\partial \boldsymbol{y}}{\partial t} \cdot \boldsymbol{d}_i = \frac{\partial y_i}{\partial t} + (\omega \times \boldsymbol{y}) \cdot \boldsymbol{d}_i \qquad (i = 1,2,3). \tag{2.4}$$

for all $s \in [a,b]$, $\forall t \geq 0$.

(b) In contrast show that the Darboux vector $\boldsymbol{u}$ and the angular velocity ω have the special properties

$$\frac{\partial \boldsymbol{u}}{\partial s} \cdot \boldsymbol{d}_i = \frac{\partial u_i}{\partial s} \qquad (i = 1,2,3), \tag{2.5}$$

$$\frac{\partial \omega}{\partial t} \cdot \boldsymbol{d}_i = \frac{\partial \omega_i}{\partial t} \qquad (i = 1,2,3). \tag{2.6}$$

for all $s \in [a,b]$, $\forall t \geq 0$.
That is, the space derivative of the component of the Darboux vector $\boldsymbol{u}$ is just the component of the space derivative of $\boldsymbol{u}$. Analogously, the time derivative of the component of the angular velocity ω is just the component of the time derivative of ω.

(c) Assuming smoothness, show further that the space derivative of the angular velocity is related to the time derivative of the Darboux vector through the relation

$$\frac{\partial \omega}{\partial s} - \frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{u} \times \omega \tag{2.7}$$

$s \in [a, b]$, $\forall t \geq 0$.

(Hint: Compute $\frac{\partial^2 \boldsymbol{d}_i}{\partial t \partial s}$ and $\frac{\partial^2 \boldsymbol{d}_i}{\partial s \partial t}$.)