DNA Modelling Course
Exercise Session 3
Summer 2006 Part 2

SOLUTIONS

Problem 1: Writhe of a curve on a sphere.

Let $\boldsymbol{x}$ be a curve on the sphere without self-intersections. Define

$$\boldsymbol{d}_1 = \frac{\boldsymbol{x}}{|\boldsymbol{x}|}, \quad \boldsymbol{d}_3 = \boldsymbol{x}' \quad \text{and} \quad \boldsymbol{d}_2 = \boldsymbol{d}_3 \times \boldsymbol{d}_1.$$

Then

$$u_3 \equiv \boldsymbol{d}_1' \cdot \boldsymbol{d}_2 = \left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right)' \cdot \left(\boldsymbol{x}' \times \frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right) = \left(\frac{\boldsymbol{x}'\,|\boldsymbol{x}| - \boldsymbol{x}\,(|\boldsymbol{x}|)'}{|\boldsymbol{x}|^2}\right) \cdot \left(\boldsymbol{x}' \times \frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right) = 0,$$

as $\boldsymbol{d}_2 = \boldsymbol{x}' \times \frac{\boldsymbol{x}}{|\boldsymbol{x}|}$ is perpendicular to both, $\boldsymbol{x}'$ and $\boldsymbol{x}$. Now we conclude

$$\begin{aligned} Wr(\boldsymbol{x}) &= Lk(\boldsymbol{x}, \boldsymbol{x} + \epsilon \boldsymbol{d}_1) - Tw(\boldsymbol{x}) \\ &= Lk(\boldsymbol{x}, \boldsymbol{x} + \epsilon \boldsymbol{d}_1) - \frac{1}{2\pi} \int_0^L u_3(s) ds = 0 - 0 = 0, \end{aligned}$$

because the link $Lk(\boldsymbol{x}, \boldsymbol{x} + \epsilon \boldsymbol{d}_1)$ is zero. (The sphere of radius $|\boldsymbol{x}| + \frac{1}{2}\epsilon$ separates the two curves $\boldsymbol{x}$ and $\boldsymbol{y} = \boldsymbol{x} + \epsilon \boldsymbol{d}_1$, so $\boldsymbol{y}$ can be dilated to infinity and therefore $Lk(\boldsymbol{x}, \boldsymbol{y}) = 0$, see Exercise Session 1, Problem 2.)

Problem 2: Inversion in a sphere.

The inversion I_σ can be written as

$$I_\sigma = T_{+\boldsymbol{c}} \circ I_{T_{-\boldsymbol{c}}(\sigma)} \circ T_{-\boldsymbol{c}},$$

where $T_{\boldsymbol{b}}$ denotes the translation $T_{\boldsymbol{b}}(\boldsymbol{x}) = \boldsymbol{x} + \boldsymbol{b}$, for $\boldsymbol{x} \in \mathbb{R}^3$. Therefore it suffices to consider inversions in spheres centred in the origin.

(a) Easy.

(b) A sphere Σ can be written in the form

$$\Sigma : \quad s_0 |\boldsymbol{x}|^2 + 2\boldsymbol{s} \cdot \boldsymbol{x} + s_4 = 0, \tag{0.1}$$

where $(s_0, \boldsymbol{s}, s_4) = (s_0, s_1, s_2, s_3, s_4) \in \mathbb{R}^5$, which are defined up to an arbitrary factor.
If $s_0 = 0$, then Σ is a plane.

Now set $\boldsymbol{y} = I_\sigma(\boldsymbol{x})$ and then $\boldsymbol{x} = I_\sigma^2(\boldsymbol{x}) = I_\sigma(\boldsymbol{y})$. Insert this into the equation (0.1), then

$$s_4|\boldsymbol{y}|^2 + 2a^2\boldsymbol{s}\cdot\boldsymbol{y} + a^4 s_0 = 0,$$

which is the equation of a sphere. Therefore $I_\sigma(\Sigma)$ is a sphere.

A circle C is the intersection of two spheres, that is $C = \sigma_1 \cap \sigma_2$. As I_σ is bijective, $I_\sigma(C) = I_\sigma(\sigma_1) \cap I_\sigma(\sigma_2)$ is again a circle.

(c) Denote the point where the two curves intersect by $\boldsymbol{p}$. If $\boldsymbol{p} \notin \sigma$, then any direction, i.e. any tangent can be described as the tangent of a circle passing through $\boldsymbol{p}$ and $I_\sigma(\boldsymbol{p})$.
We therefore have two circles σ_1, σ_2, each passing through $\boldsymbol{p}$ and $I_\sigma(\boldsymbol{p})$, that intersect in the same directions as the two curves. It holds $I_\sigma(\sigma_i) = \sigma_i$, $i = 1, 2$ (as $I_\sigma(\boldsymbol{p}), \boldsymbol{p} = I_\sigma(I_\sigma(\boldsymbol{p}))$ and the two intersection points with σ are element of $I_\sigma(\sigma_i) \cap \sigma_i$). By symmetry (reflection i n the plane in the middle and perpendicular to the segment $\boldsymbol{p}, I_\sigma(\boldsymbol{p})$) the angle at $I_\sigma(\boldsymbol{p})$ is the same as the angle at $\boldsymbol{p}$.
If $\boldsymbol{p} \in \sigma$, then write I_σ =dilatation$\circ I_{\bar\sigma}$, such that $\boldsymbol{p} \notin \bar\sigma$ and $\bar\sigma, \sigma$ are concentric spheres. A dilatation keeps angles invariant, $I_{\bar\sigma}$ keeps angles invariant as seen above.

Problem 3: Total Twist under inversions.

Let $\boldsymbol{x}$ be a curve and I_σ the inversion in a sphere of radius a and center $\boldsymbol{c}$, that is

$$I_\sigma : \boldsymbol{x} \to \boldsymbol{c} + \frac{a^2}{|\boldsymbol{x}-\boldsymbol{c}|^2}(\boldsymbol{x}-\boldsymbol{c}), \quad I_\sigma(\boldsymbol{c}) = \infty, \quad I_\sigma(\infty) = \boldsymbol{c}.$$

The inversion I_σ is a conformal transformation, that is, I_σ keeps angles between curves invariant.
Let $\boldsymbol{d}$ be a unit vector field along $\boldsymbol{x}$. The oriented straight line generated by $\boldsymbol{d}$ is mapped by I_σ into an oriented circle. The tangent to this circle will be denoted by $\bar{\boldsymbol{d}}$. Then

$$\begin{aligned}\bar{\boldsymbol{d}} &= \boldsymbol{d} - \frac{2\boldsymbol{d}\cdot(\boldsymbol{x}-\boldsymbol{c})}{(\boldsymbol{x}-\boldsymbol{c})\cdot(\boldsymbol{x}-\boldsymbol{c})}(\boldsymbol{x}-\boldsymbol{c}) = \left[id - 2\frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|} \circ \left(\frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|}\right)^t\right]\boldsymbol{d} \\ &= \left[id - 2\frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|} \otimes \frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|}\right]\boldsymbol{d} = R\boldsymbol{d}.\end{aligned} \tag{0.2}$$

The conformal mapping I_σ transforms the orthonormal frame $(\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3)$ into orthonormal frame $(\bar{\boldsymbol{d}}_1, \bar{\boldsymbol{d}}_2, \bar{\boldsymbol{d}}_3)$. But I_σ changes the orientation of the base.

The matrix R has determinant -1, because it has the eigenvalues $1, 1, -1$ with the corresponding eigenvectors

$$\boldsymbol{e}, \quad (\boldsymbol{x}-\boldsymbol{c}) \times \boldsymbol{e} \quad \text{and} \quad \frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|}.$$

where $\boldsymbol{e}$ is a vector perpendicular to $(\boldsymbol{x}-\boldsymbol{c})$. And so we see that

$$|\bar{\boldsymbol{d}}_1\bar{\boldsymbol{d}}_2\bar{\boldsymbol{d}}_3| = |R \circ [\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_3]| = |R|\,|\boldsymbol{d}_1\boldsymbol{d}_2\boldsymbol{d}_3| = -1,$$

thus $(\bar{\boldsymbol{d}}_1, -\bar{\boldsymbol{d}}_2, \bar{\boldsymbol{d}}_3)$ is a right-handed orthonormal base, given that $(\boldsymbol{d}_1, \boldsymbol{d}_2, \boldsymbol{d}_3)$ was a right-handed orthonormal base.
Using the formula (0.2) we derive

$$\frac{\delta \boldsymbol{d}_1}{\delta s} \cdot \boldsymbol{d}_2 = \frac{\delta \bar{\boldsymbol{d}}_1}{\delta s} \cdot \bar{\boldsymbol{d}}_2.$$

Furthermore I_σ maps the tangent $\boldsymbol{d}_3$ to the curve $\boldsymbol{x}$ into $\bar{\boldsymbol{d}}_3$ which is a tangent to the curve $I_\sigma \boldsymbol{x}$. Indeed

$$\begin{aligned}(I_\sigma \boldsymbol{x})' = DI_\sigma \circ \boldsymbol{x}' &= \frac{a^2}{|\boldsymbol{x}-\boldsymbol{c}|^2}\left[id - 2\frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|} \circ \left(\frac{\boldsymbol{x}-\boldsymbol{c}}{|\boldsymbol{x}-\boldsymbol{c}|}\right)^t\right] \circ \boldsymbol{x}' \\ &= \frac{a^2}{|\boldsymbol{x}-\boldsymbol{c}|^2} R \circ \boldsymbol{d}_3 = \frac{a^2}{|\boldsymbol{x}-\boldsymbol{c}|^2}\bar{\boldsymbol{d}}_3.\end{aligned}$$

We denote by $\tilde{u}$ the Darboux vector corresponding to $(\bar{\boldsymbol{d}}_1, -\bar{\boldsymbol{d}}_2, \bar{\boldsymbol{d}}_3)$. Then we have $\bar{u}_3 = \tilde{u} \cdot \bar{\boldsymbol{d}}_3 = \frac{\delta \bar{\boldsymbol{d}}_1}{\delta s} \cdot (-\bar{\boldsymbol{d}}_2)$. Now we get

$$\begin{aligned} Tw(I\boldsymbol{x}, \bar{\boldsymbol{d}}_1) &= \frac{1}{2\pi}\int_0^L \bar{u}_3\, ds = \frac{1}{2\pi}\int_0^L \frac{\delta \bar{\boldsymbol{d}}_1}{\delta s} \cdot (-\bar{\boldsymbol{d}}_2)\, ds \\ &= -\frac{1}{2\pi}\int_0^L \frac{\delta \boldsymbol{d}_1}{\delta s} \cdot \boldsymbol{d}_2\, ds = -\frac{1}{2\pi}\int_0^L u_3\, ds = -Tw(\boldsymbol{x}, \boldsymbol{d}_1).\end{aligned}$$

Problem 4: General form of the Darboux vector of an adapted framing of a given curve.

1. We calculate
$$\frac{d}{ds}|\boldsymbol{\xi}(s)|^2 = 2\boldsymbol{\xi}(s) \cdot \boldsymbol{\xi}'(s) = 0$$
Therefore $|\boldsymbol{\xi}(s)|^2$ is constant. From the initial value we get $|\boldsymbol{\xi}(s)|^2 = 1$ for all s.

2. Now we derive
$$\begin{aligned}\frac{d}{ds}(\boldsymbol{\xi} \cdot \boldsymbol{r}') &= ((u_3(s)\boldsymbol{r}' + \boldsymbol{r}' \times \boldsymbol{r}'') \times \boldsymbol{\xi}) \cdot \boldsymbol{r}' + \boldsymbol{\xi} \cdot \boldsymbol{r}'' \\ &= ((\boldsymbol{r}' \times \boldsymbol{r}'') \times \boldsymbol{\xi}) \cdot \boldsymbol{r}' + \boldsymbol{\xi} \cdot \boldsymbol{r}'' \\ &= ((\boldsymbol{r}' \cdot \boldsymbol{\xi})\boldsymbol{r}'' - (\boldsymbol{r}'' \cdot \boldsymbol{\xi})\boldsymbol{r}') \cdot \boldsymbol{r}' + \boldsymbol{\xi} \cdot \boldsymbol{r}'' = (\boldsymbol{r}' \cdot \boldsymbol{\xi})(\boldsymbol{r}'' \cdot \boldsymbol{r}') = 0.\end{aligned}$$
The vector $\boldsymbol{\xi}(s)$ is perpendicular to $\boldsymbol{r}'(s)$ for all s.

3. Now by picking an initial value of $\boldsymbol{\xi}(0)$ we have an orthonormal frame $(\boldsymbol{\xi}, \boldsymbol{r}' \times \boldsymbol{\xi}, \boldsymbol{r}')$ of $\boldsymbol{r}(s)$.
   The Darboux vector is $u_3(s)\boldsymbol{r}' + \boldsymbol{r}' \times \boldsymbol{r}''$. This is the general form of a Darboux vector. To verify we calculate

$$\begin{aligned}(u_3\boldsymbol{r}' + \boldsymbol{r}' \times \boldsymbol{r}'') \times \boldsymbol{r}' &= (\boldsymbol{r}' \times \boldsymbol{r}'') \times \boldsymbol{r}' = \boldsymbol{r}'' \\ (u_3\boldsymbol{r}' + \boldsymbol{r}' \times \boldsymbol{r}'') \times (\boldsymbol{r}' \times \boldsymbol{\xi}) &= -u_3\boldsymbol{\xi} + (\boldsymbol{r}' \times \boldsymbol{r}'') \times (\boldsymbol{r}' \times \boldsymbol{\xi}) \\ &= -u_3\boldsymbol{\xi} + \boldsymbol{r}'' \times \boldsymbol{\xi} = (\boldsymbol{r}' \times \boldsymbol{\xi})'.\end{aligned}$$

4. This is the fact that $u_3(s)\boldsymbol{r}' + \boldsymbol{r}' \times \boldsymbol{r}''$ is the Darboux vector corresponding to the frame $(\boldsymbol{\xi}, \boldsymbol{r}' \times \boldsymbol{\xi}, \boldsymbol{r}')$. The concrete calculation is the same as in (c).

5. If $\boldsymbol{r}'' \neq 0$ then $\boldsymbol{r}' \times \boldsymbol{r}'' = \kappa \boldsymbol{b}$ and therefore the Darboux vector is

$$u_3\boldsymbol{t} + \kappa\boldsymbol{b}$$

   where $\boldsymbol{t} = \boldsymbol{r}'$, $\boldsymbol{n} = \frac{r''}{|r''|}, \kappa = |\boldsymbol{r}''|$, $\boldsymbol{b} = \boldsymbol{t} \times \boldsymbol{n}$.

Problem 5: Self-link of a curve on a sphere.

1. Link is invariant under translations and dilatations, therefore we may assume, the sphere is the unit sphere. Then

$$\boldsymbol{r} \cdot \boldsymbol{r} = 1 \quad \Rightarrow \quad \boldsymbol{r} \cdot \boldsymbol{r}' = 0 \quad \Rightarrow \quad \boldsymbol{r} \cdot \boldsymbol{r}'' = -1 \quad \Rightarrow \quad \boldsymbol{r} \cdot \boldsymbol{n} = \frac{-1}{\kappa}.$$

   The curve $\boldsymbol{r}$ is smooth and defined on a compact inverval, therefore we get

$$\boldsymbol{r} \cdot \boldsymbol{n} = \frac{-1}{\kappa} < -\delta < 0.$$

   for some constant $\delta < 0$. For a small $\varepsilon > 0$ the second curve $\boldsymbol{y} = \boldsymbol{r} + \varepsilon\boldsymbol{n}$ can be separated by a sphere from the curve $\boldsymbol{r}$ lying on the unit sphere. Using invariance under smooth deformations (with the non-intersection property) of the Link we see that the self-link is zero, i.e. $SLk(\boldsymbol{r}) = Lk(\boldsymbol{r}, \boldsymbol{r} + \varepsilon\boldsymbol{n}) = 0$.

2. From Problem 1 we know that the Writhe of $\boldsymbol{r}$ is zero. From the Calugareanu-Fuller-White formula we conclude that the Twist $Tw(\boldsymbol{r}) = \frac{1}{2\pi}\int \tau(s)ds$ is zero.