DNA Modelling Course
Exercise Session 5
Summer 2006 Part 1

SOLUTIONS

1 Equilibrium configurations for a system of two rigid bars

(a) Equilibria for the current system are critical points of the energy function

$$E(\theta,\phi,\lambda)=\frac{1}{2}\theta^2+\frac{1}{2}(\theta-\phi)^2+\lambda(\cos\theta+\cos\phi). \tag{1.1}$$

Thus, equilibria satisfy the equations

$$\left.\begin{array}{rclcl}\frac{\partial E}{\partial\theta} &=& 2\theta-\phi-\lambda\sin\theta &=& 0\\ \frac{\partial E}{\partial\phi} &=& -\theta+\phi-\lambda\sin\phi &=& 0\end{array}\right\} \tag{1.2}$$

and clearly $(\theta_0,\phi_0)=(0,0)$ is an equilibrium for any $\lambda>0$.

(b) The function we will use for the Implicit function theorem, is the function $\boldsymbol{F}:\mathbb{R}^2\times\mathbb{R}\to\mathbb{R}^2$ defined as follows

$$\boldsymbol{F}(\theta,\phi,\lambda)=\left\{\begin{array}{ll}F_1(\theta,\phi,\lambda) &=\frac{\partial E}{\partial\theta},\\ F_2(\theta,\phi,\lambda) &=\frac{\partial E}{\partial\phi}.\end{array}\right.$$

Having said this, as by construction $\boldsymbol{F}(\theta_0,\phi_0,\lambda_0)=\boldsymbol{F}(0,0,\lambda_0)=0$ (this is true for each λ_0, so you can fix an arbitrary λ_0), the only thing to check is weather and under which conditions the following Jacobian matrix is singular

$$\begin{aligned}\boldsymbol{J_F}(\theta_0,\phi_0,\lambda_0) &= \begin{pmatrix}\frac{\partial F_1}{\partial\theta} & \frac{\partial F_1}{\partial\phi}\\ \frac{\partial F_2}{\partial\theta} & \frac{\partial F_2}{\partial\phi}\end{pmatrix}(0,0,\lambda_0)\\ &= \begin{pmatrix}2-\lambda_0 & -1\\ -1 & 1-\lambda_0\end{pmatrix}.\end{aligned} \tag{1.3}$$

This matrix is invertible (i.e. non singular) if and only if $\det(\boldsymbol{J_F})\neq 0$, that is for $\lambda_0\neq(3\mp\sqrt{5})/2$. In conclusion then, the Implicit function theorem guarantees that for each $\lambda_0\neq(3\mp\sqrt{5})/2$ in a neighborhood

$\tilde{U}(0,0,\lambda_0) = U(0,0) \times V(\lambda_0)$, there exists a unique $\Theta(\lambda) = (\theta(\lambda), \phi(\lambda))$ with

$$\begin{aligned} \boldsymbol{F}(\Theta(\lambda), \lambda) &= 0 \\ \Theta(\lambda_0) &= (0,0). \end{aligned} \tag{1.4}$$

Finally, since we already know a solution of $\boldsymbol{F}(\theta, \phi, \lambda) = 0$, which is the trivial solution $(\theta(\lambda), \phi(\lambda), \lambda) = (0, 0, \lambda)$ (i.e. the function $\Theta(\lambda)$ is just $(0,0)\ \forall\lambda$), we can conclude that *it is the only* solution!! It is important to note that the theorem is only a local theorem! The only definitive statement here is that there exist two points (two values of the parameter λ) where the Implicit function theorem cannot be applied and where we expect to find other solutions different from the trivial one. In order to understand in details what happens around the trivial solution and *at* the parameter values $\lambda = (3 \mp \sqrt{5})/2$ we will need to use a perturbation expansion tecnique (see next exercise session).

(c) For each of the two values $\lambda = \lambda_0^{(i)}$, where $\lambda_0^{(1)} = (3 - \sqrt{5})/2$ and $\lambda_0^{(2)} = (3 + \sqrt{5})/2$, the null space of $\boldsymbol{J_F}$ is one-dimensional and

$$\mathcal{N}[\boldsymbol{J_F}] = \text{span}\{(1, 2 - \lambda)\}.$$

More precisely we have

$$\mathcal{N}[\boldsymbol{J_F}(\lambda_0^{(1)})] = \text{span}\{(1, \frac{1+\sqrt{5}}{2})\} \tag{1.5}$$

where both components are positive and

$$\mathcal{N}[\boldsymbol{J_F}(\lambda_0^{(2)})] = \text{span}\{(1, \frac{1-\sqrt{5}}{2})\} \tag{1.6}$$

where one component is positive, the other is negative. Usually one indicates the normalized vectors spanning the null space. Here (two dimensions) we take the first component to be one, then the calcuations become a bit easier.

2 Stability

(a) By definition, the Hessian of $E(\theta, \phi)$ is the symmetric matrix function

$$\text{hess}[E](\theta, \phi) = \begin{pmatrix} \frac{\partial^2 E}{\partial \theta^2} & \frac{\partial^2 E}{\partial \phi \partial \theta} \\ \frac{\partial^2 E}{\partial \theta \partial \phi} & \frac{\partial^2 E}{\partial \phi^2} \end{pmatrix} = \begin{pmatrix} 2 - \lambda \cos\theta & -1 \\ -1 & 1 - \lambda\cos\theta \end{pmatrix}, \tag{2.1}$$

and at the equilibria $(\theta_0, \phi_0, \lambda_0) = (0, 0, \lambda_0)$ we have

$$\text{hess}[E](\theta_0, \phi_0) = \begin{pmatrix} 2 - \lambda_0 & -1 \\ -1 & 1 - \lambda_0 \end{pmatrix}. \tag{2.2}$$

The signs of the eigenvalues μ_i $(i = 1, 2)$ of $\text{hess}[E](\theta_0, \phi_0)$ determine whether the critical point (θ_0, ϕ_0) is a local minima (both positive), maxima (both negative), saddle (one positive, negative) or degenerate (at least one zero). Using the facts

$$\left.\begin{array}{lclcl} \mu_1\mu_2 & = & \det[\text{hess}[E](\theta_0, \phi_0)] & = & \lambda_0^2 - 3\lambda_0 + 1 \\ \mu_1 + \mu_2 & = & \text{tr}[\text{hess}[E](\theta_0, \phi_0)] & = & 3 - 2\lambda_0, \end{array}\right\} \tag{2.3}$$

we find that (θ_0, ϕ_0) is a

$$\left.\begin{array}{lll} \text{local minima} & \text{if} & 0 < \lambda_0 < \frac{3-\sqrt{5}}{2} \\ \text{local saddle} & \text{if} & \frac{3-\sqrt{5}}{2} < \lambda_0 < \frac{3+\sqrt{5}}{2} \\ \text{local maxima} & \text{if} & \frac{3+\sqrt{5}}{2} < \lambda_0 < \infty \\ \text{degenerate} & \text{if} & \lambda_0 = \frac{3-\sqrt{5}}{2}, \frac{3+\sqrt{5}}{2}. \end{array}\right\} \tag{2.4}$$

Note that changes in stability are exactly at points where the $\boldsymbol{J_F}$ (which is by construction $\text{hess}[E]$!!) is degenerate (i.e. points where the Implicit function theorem cannot be applied), i.e. at *bifurcation* points.