MATH 728A, BIOMOLECULAR GEOMETRY, SOLUTION TO HOMEWORK 7.1

Problem 7.1 (Rotation Matrices). Define SO(3) to be the set of all rotation matrices A, i.e. 3×3 real matrices such that $A^T A = I$ (I denotes the 3×3 identity matrix) and $\det A = 1$. Show that there exists a pair $(e^{i\theta}, \mathbf{u})$, uniquely determined (when $A \neq I$) up to reflection $(e^{-i\theta}, -\mathbf{u})$, where θ is real and $\mathbf{u} \in \mathbb{R}^3$ is a unit vector, such that for all $\mathbf{x} \in \mathbb{R}^3$ we have

$$A\mathbf{x} = \mathbf{u}(\mathbf{u} \cdot \mathbf{x}) + [\mathbf{x} - \mathbf{u}(\mathbf{u} \cdot \mathbf{x})] \cos\theta + (\mathbf{u} \times \mathbf{x}) \sin\theta.$$

Solution. First we will prove the following Lemma:

Lemma. *If $A \in SO(3)$ then there exists a matrix $U \in SO(3)$ such that $AU = UR$, where*

$$R = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad 0 \leq \theta \leq \pi.$$

The third column of the matrix U is the axis of the right-handed rotation through the angle θ performed by A in $\mathbb{R}^3$.

Proof. If $x, y \in \mathbb{R}^3$ then $(Ax)^T Ay = x^T A^T Ay = x^T y$, so in particular $\|Ax\| = \|x\|$ and the angle between Ax and Ay is the same as the angle between x and y. The cubic polynomial $\det(\lambda I - A)$ has real coefficients, so A has at least one real eigenvalue, and any nonreal eigenvalues must form a complex conjugate pair. If λ is any eigenvalue of A with eigenvector x, then $\|Ax\| = \|x\|$ implies $|\lambda| = 1$. Thus the real eigenvalues are from the set $\{1, -1\}$. If -1 is the only real eigenvalue, it cannot occur with algebraic multiplicity two, since the other eigenvalue would have to be real, and yet could not be 1 or -1. Since $\det(A)$ is the product of the eigenvalues, we see that the product of the eigenvalues is 1. If -1 has multiplicity one, then there must be a nonreal complex conjugate pair $e^{i\theta}, e^{-i\theta}$ of eigenvalues. But since the product of $e^{i\theta}$ and its complex conjugate is 1, we obtain the contradiction that $(-1)e^{i\theta}e^{-i\theta} = 1$. If -1 has multiplicity three then we obtain the contradiction $(-1)^3 = 1$. Thus 1 must be an eigenvalue. Let $\tilde{u}_3$ be a normalized eigenvector of A belonging to the eigenvalue 1, and let $\tilde{u}_1, \tilde{u}_2$ be an orthonormal basis of the plane perpendicular to $\tilde{u}_3$, so that $(\tilde{u}_1, \tilde{u}_2, \tilde{u}_3)$ forms a positively oriented frame of $\mathbb{R}^3$. Define

$$(u_1, u_2, u_3) = \begin{cases} (\tilde{u}_1, \tilde{u}_2, \tilde{u}_3) & \tilde{u}_2^T A \tilde{u}_1 \geq 0, \\ (\tilde{u}_2, \tilde{u}_1, -\tilde{u}_3) & \tilde{u}_2^T A \tilde{u}_1 < 0. \end{cases}$$

Clearly (u_1, u_2, u_3) is a positively oriented orthonormal basis. In the first case above we clearly have $u_2^T A u_1 \geq 0$. In the second case we claim that $u_2^T A u_1 > 0$. To see this, let $P = \operatorname{span}\{u_1, u_2\}$. A maps P into itself. The ordered pairs (u_1, u_2) and (Au_1, Au_2)

determine the same orientation of P, i.e. they are related by a 2×2 matrix with positive determinant. (To see this note that

$$A(u_1, u_2, u_3) = (Au_1, Au_2, Au_3) = (u_1, u_2, u_3) \begin{pmatrix} a_{11} & a_{21} & 0 \\ a_{12} & a_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Now take the determinant of both sides of this equation.) Let the plane P be coordinatized by the components with respect to the vectors $(\tilde{u}_1, \tilde{u}_2)$. Then the second case is characterized by the inequality $\tilde{u}_2^T A\tilde{u}_1 < 0$, which means that $Au_2 = A\tilde{u}_1$ is in the third or fourth quadrant. Hence $Au_1 = A\tilde{u}_2$ is in the first or fourth quadrant, and hence the angle between u_2 and Au_1 is less than $\pi/2$, as claimed. Now define $0 \le \theta \le \pi$ such that $\cos\theta = u_1^T Au_1$. It follows that $Au_1 = u_1 \cos\theta + u_2 \sin\theta$ and $Au_2 = u_1(-\sin\theta) + u_2 \cos\theta$. Setting $U = (u_1, u_2, u_3)$ we get the result. $\square$

We define $\mathbf{u}$ to be the third column vector u_3 of the matrix U in the above lemma. Now let $\mathbf{x} \in \mathbb{R}^3$ be given. Since $U \in SO(3)$ we have $U^{-1} = U^T$. Thus

$$\begin{aligned} A\mathbf{x} = URU^T\mathbf{x} &= \begin{pmatrix} u_1 & u_2 & \mathbf{u} \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1^T\mathbf{x} \\ u_2^T\mathbf{x} \\ \mathbf{u}^T\mathbf{x} \end{pmatrix} \\ &= \begin{pmatrix} u_1 & u_2 & \mathbf{u} \end{pmatrix} \begin{pmatrix} \cos\theta u_1^T\mathbf{x} - \sin\theta u_2^T\mathbf{x} \\ \sin\theta u_1^T\mathbf{x} + \cos\theta u_2^T\mathbf{x} \\ \mathbf{u}^T\mathbf{x} \end{pmatrix} \\ &= u_1(\cos\theta u_1^T\mathbf{x} - \sin\theta u_2^T\mathbf{x}) + u_2(\sin\theta u_1^T\mathbf{x} + \cos\theta u_2^T\mathbf{x}) + \mathbf{u}\mathbf{u}^T x \\ &= \mathbf{u}\mathbf{u}^T x + (u_1 u_1^T\mathbf{x} + u_2 u_2^T\mathbf{x})\cos\theta + (-u_1 u_2^T\mathbf{x} + u_2 u_1^T\mathbf{x})\sin\theta. \end{aligned}$$

Since $I = UU^T = u_1u_1^T + u_2u_2^T + \mathbf{u}\mathbf{u}^T$ we have that $u_1u_1^T + u_2u_2^T = I - \mathbf{u}\mathbf{u}^T$ and therefore $u_1u_1^T\mathbf{x} + u_2u_2^T\mathbf{x} = \mathbf{x} - \mathbf{u}\mathbf{u}^T\mathbf{x}$. Also $\mathbf{u} \times \mathbf{x} = \mathbf{u} \times (u_1u_1^T\mathbf{x} + u_2u_2^T\mathbf{x} + \mathbf{u}\mathbf{u}^T\mathbf{x}) = (\mathbf{u} \times u_1)u_1^T\mathbf{x} + (\mathbf{u} \times u_2)u_2^T\mathbf{x} = u_2u_1^T\mathbf{x} - u_1u_2^T\mathbf{x}$. This demonstrates the existence of the pair $(e^{i\theta}, \mathbf{u})$ with the desired properties.

Clearly if the pair $(e^{i\theta}, \mathbf{u})$ works then so does $(e^{-i\theta}, -\mathbf{u})$. The vector $\mathbf{u}$ must be an eigenvector of A associated to the eigenvalue 1, and this eigenvalue cannot have algebraic or geometric multiplicity two, since then the other eigenvalue would have to be -1, contradicting the fact that $\det A = 1$. (The geometric multiplicity is equal to the algebraic multiplicity since A is clearly diagonalizable.) If the multiplicity is 3 then $A = I$. If $A \neq I$ then the multiplicity is 1, and hence the eigenspace of 1 contains only two real unit eigenvectors. Suppose $\mathbf{x}$ is a unit vector perpendicular to $\mathbf{u}$. Then $A\mathbf{x} = \mathbf{x}\cos\theta + \mathbf{u} \times \mathbf{x}\sin\theta$ is an expansion in an orthonormal basis $\{\mathbf{u}, \mathbf{x}, \mathbf{u} \times \mathbf{x}\}$, and hence $\cos\theta = \mathbf{x} \cdot A\mathbf{x}$ and $\sin\theta = (\mathbf{u} \times \mathbf{x}) \cdot A\mathbf{x}$. The same values of $\cos\theta$ and $\sin\theta$ are obtained independently of the choice of $\mathbf{x}$. Thus both $\cos\theta$ and $\sin\theta$ are determined by $\mathbf{u}$. This proves the uniqueness claim.