3.3.1.2.3. *Orthogonalization of impure rotations*

There are several ways of deriving a strictly orthogonal matrix from a given approximately orthogonal matrix, among them the following.

(i) The Gram–Schmidt process. This is probably the simplest and the easiest to compute. If the given matrix consists of three column vectors $\mathbf{v}_1, \mathbf{v}_2$ and $\mathbf{v}_3$ (later referred to as primers) which are to be replaced by three column vectors $\mathbf{u}_1, \mathbf{u}_2$ and $\mathbf{u}_3$ then the process is

$$\begin{aligned}\mathbf{u}_1 &= \mathbf{v}_1/|\mathbf{v}_1| \\ \mathbf{u}_2 &= \mathbf{v}_2 - (\mathbf{u}_1 \cdot \mathbf{v}_2)\mathbf{u}_1 \\ \mathbf{u}_2 &= \mathbf{u}_2/|\mathbf{u}_2| \\ \mathbf{u}_3 &= \mathbf{v}_3 - (\mathbf{u}_1 \cdot \mathbf{v}_3)\mathbf{u}_1 - (\mathbf{u}_2 \cdot \mathbf{v}_3)\mathbf{u}_2 \\ \mathbf{u}_3 &= \mathbf{u}_3/|\mathbf{u}_3|.\end{aligned}$$

As successive vectors are established, each vector $\mathbf{v}$ has subtracted from it its components in the directions of established vectors, and the remainder is normalized. The method will fail at the normalization step if the vectors $\mathbf{v}$ are not linearly independent. Otherwise, the process may be extended to any number of dimensions.

The weakness of the method is that, though $\mathbf{u}_1$ differs from $\mathbf{v}_1$ only in scale, $\mathbf{u}_N$ may differ grossly from $\mathbf{v}_N$ as the various columns are not treated equivalently.

(ii) A preferable method which treats all vectors equivalently is to iteratively replace the matrix $\boldsymbol{M}$ by $\frac{1}{2}(\boldsymbol{M} + \boldsymbol{M}^{T-1})$.

Defining the residual matrix $\boldsymbol{E}$ as

$$\boldsymbol{E} = \boldsymbol{M}\boldsymbol{M}^T - \boldsymbol{I},$$

then on each iteration $\boldsymbol{E}$ is replaced by

$$\boldsymbol{E}^2(\boldsymbol{M}\boldsymbol{M}^T)^{-1}/4$$

and convergence necessarily ensues.

(iii) A third method resolves $\boldsymbol{M}$ into its symmetric and antisymmetric parts

$$\boldsymbol{S} = \tfrac{1}{2}(\boldsymbol{M} + \boldsymbol{M}^T), \quad \boldsymbol{A} = \tfrac{1}{2}(\boldsymbol{M} - \boldsymbol{M}^T), \quad \boldsymbol{M} = \boldsymbol{S} + \boldsymbol{A}$$

and constructs an orthogonal matrix for which only $\boldsymbol{S}$ is altered. $\boldsymbol{A}$ determines l, m, n and θ as shown in Section 3.3.1.2.1, and from these a new $\boldsymbol{S}$ may be constructed.

(iv) A fourth method is to treat the general matrix $\boldsymbol{M}$ as a combination of pure strain and pure rotation. Setting

$$\boldsymbol{M} = \boldsymbol{R}\boldsymbol{T}$$

with $\boldsymbol{R}$ orthogonal and $\boldsymbol{T}$ symmetrical gives

$$\boldsymbol{T} = (\boldsymbol{M}^T\boldsymbol{M})^{1/2}, \quad \boldsymbol{R} = \boldsymbol{M}(\boldsymbol{M}^T\boldsymbol{M})^{-1/2}.$$

The rotation so found is the one which exactly superposes those three mutually perpendicular directions which remain mutually perpendicular under the transformation $\boldsymbol{M}$.

$\boldsymbol{T} - \boldsymbol{I}$ is then the strain tensor of an unrotated body.

Writing $\boldsymbol{M} = \boldsymbol{T}\boldsymbol{R}$, $\boldsymbol{T} = (\boldsymbol{M}\boldsymbol{M}^T)^{1/2}$, $\boldsymbol{R} = (\boldsymbol{M}\boldsymbol{M}^T)^{-1/2}\boldsymbol{M}$ may also be useful, in which $\boldsymbol{T} - \boldsymbol{I}$ is the strain tensor of a rotated body. See also Section 3.3.1.2.2 (iv).

3.3.1.2.4. *Eigenvalues and eigenvectors of orthogonal matrices*

If $\boldsymbol{R}$ is the orthogonal matrix given in Section 3.3.1.2.1 in terms of the direction cosines l, m and n of the axis of rotation, then it is clear that (l, m, n) is an eigenvector of $\boldsymbol{R}$ with eigenvalue unity because

$$\boldsymbol{R}\begin{pmatrix} l \\ m \\ n \end{pmatrix} = \begin{pmatrix} l \\ m \\ n \end{pmatrix}.$$

Consideration of the determinant $|\boldsymbol{R} - \lambda\boldsymbol{I}| = 0$ shows that the sum of the three eigenvalues is $1 + 2\cos\theta$ and that their product is unity. Hence the three eigenvalues are 1, $e^{i\theta}$ and $e^{-i\theta}$. Since $\boldsymbol{R}$ is real, its product with any real vector is also real, yet its product with an eigenvector must, in general, be complex. Thus the eigenvectors must themselves be complex.

The remaining two eigenvectors $\mathbf{u}$ may be found using the results of Section 3.3.1.2.1 (*q.v.*) according to

$$\boldsymbol{R}\mathbf{u} = \mathbf{u} + \frac{2}{1+t^2}\{(\mathbf{r} \times \mathbf{u}) + [\mathbf{r} \times (\mathbf{r} \times \mathbf{u})]\} = \mathbf{u}e^{\pm i\theta} = \mathbf{u}\frac{1 \pm it}{1 \mp it},$$

which is solved by any vector of the form

$$\mathbf{u} = \mathbf{l} \times \mathbf{v} \mp i\mathbf{l} \times (\mathbf{l} \times \mathbf{v})$$

for any real vector $\mathbf{v}$, where $\mathbf{l}$ is the normalized axis vector, $\mathbf{l}t = \mathbf{r}$, $|\mathbf{l}| = 1$, $t = \tan(\theta/2)$. Eigenvectors for the two eigenvalues may have unrelated $\mathbf{v}$ vectors though the sign choices are coupled. If the vector $\mathbf{v}$ is rotated about $\mathbf{l}$ through an angle φ the corresponding vector $\mathbf{u}$ is multiplied by $e^{-i\varphi}$ and remains an eigenvector. Using superscript signs to denote the sign of θ in the eigenvalue with which each vector is associated, the matrix

$$\boldsymbol{U} = (\mathbf{l},\ \mathbf{u}^+,\ \mathbf{u}^-)$$

has the properties that

$$\boldsymbol{R}\boldsymbol{U} = \boldsymbol{U}\begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{i\theta} & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix}$$

and

$$\boldsymbol{U}^{*T}\boldsymbol{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2|\mathbf{l} \times \mathbf{v}^+|^2 & 0 \\ 0 & 0 & 2|\mathbf{l} \times \mathbf{v}^-|^2 \end{pmatrix}$$

which places restrictions on $\mathbf{v}$ if this is to be the identity. Note that the 23 element vanishes even in the absence of any relationship between $\mathbf{v}^+$ and $\mathbf{v}^-$.

A convenient form for $\boldsymbol{U}$, symmetrical in the elements of $\mathbf{l}$, is obtained by setting $\mathbf{v}^+ = \mathbf{v}^- = [111]$ and is

$$\boldsymbol{U} = \begin{pmatrix} l & \{(m-n) - i[l(l+m+n)-1]\}/d & \{(m-n) + i[l(l+m+n)-1]\}/d \\ m & \{(n-l) - i[m(l+m+n)-1]\}/d & \{(n-l) + i[m(l+m+n)-1]\}/d \\ n & \{(l-m) - i[n(l+m+n)-1]\}/d & \{(l-m) + i[n(l+m+n)-1]\}/d \end{pmatrix}$$

in which the normalizing denominator is given by

$$d = 2\sqrt{1 - lm - mn - nl}.$$

3.3.1.3. *Projection transformations and spaces*

In the following section we address the question of the relationship between the coordinates of a molecular model and the corresponding coordinates on the screen of the graphics device. A good introduction to this topic is given by Newman & Sproull (1973), and Foley *et al.* (1990) give a comprehensive account of the field, including recent developments, especially those arising from the development of raster-graphics technologies.

3.3.1.3.1. *Definitions*

Typically, the coordinates, $\mathbf{X}$, of points in an object to be drawn are held in homogeneous Cartesian form as described in Section 3.3.1.1.2. Such coordinates are said to be in *data space* or world

references