6. Rotations

In previous lecture we discussed orthogonal transformations and rotations in three dimensions. In this lecture we give a more formal discussion of rotations.

Orthogonal transformations leave the origin fixed and preserve all angles and distances, so they are called *rigid motions*. An orthogonal transformation is given by a 3×3 matrix and the columns of the matrix can be thought of as an orthonormal frame. The group of orthogonal matrices is called O(3).

The condition for a matrix to be orthogonal is that the entries are real and

$$\mathbf{A}'\,\mathbf{A} = \mathbf{I}. \tag{1}$$

A matrix satisfying (1) preserves the dot product since this condition implies that

$$\begin{aligned}\mathbf{Av}\cdot\mathbf{Aw} &= (\mathbf{Av})'\mathbf{Aw} = \mathbf{v}'\mathbf{A}'\mathbf{Aw}\\ &= \mathbf{v}'\mathbf{Iw} = \mathbf{v}'\mathbf{w} = \mathbf{v}\cdot\mathbf{w}.\end{aligned}$$

Thus *orthogonal transformations preserve the dot product* and hence lengths and angles, since lengths and angles can be described by dot products.

All orthogonal transformations have determinant ±1 since

$$\begin{aligned}(\det\mathbf{A})^2 &= \det(\mathbf{A}')\det\mathbf{A}\\ &= \det(\mathbf{A}'\,\mathbf{A})\\ &= \det\mathbf{I} = 1.\end{aligned}$$

6.1. **The rotation group.** Rotation matrices are orthogonal matrices whose determinant is 1. A rotation is an orthogonal transformation which preserves orientations, so the columns are a right handed frame. The determinant is the scalar triple product of the vectors in the frame and so it is positive and must be 1. The group of rotations is denoted SO(3) .

We are interested mostly in dimension three because molecules are structures in three dimensional space. A similar discussion could be given in any dimension n where the groups would be denoted O(n) and SO(n). It is often instructive to look at dimension two, since the situation is simpler and we can gain some intuition for three dimensions.

6.2. **Rotations in dimension 2.** In two dimensions, a right-handed orthonormal frame can be constructed given an angle θ by taking

$$\mathrm{R}(\theta) = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix} \tag{2}$$

and this matrix gives the frame that the standard frame

$$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

moves to under counterclockwise rotation by an angle θ. Equation (2) gives all possible rotations in two dimensions.

Rotation in two dimensions can be conveniently done using complex numbers. If $e^{i\theta} = \cos\theta + i\sin\theta$ and $z = x + iy$, the map $z \to e^{i\theta}z$ represents counterclockwise rotation an angle of θ.

Note that

$$\mathrm{R}(\theta)\mathrm{R}(\phi) = \mathrm{R}(\theta+\phi) = \mathrm{R}(\phi)\mathrm{R}(\theta),$$

so that rotations in two dimension commute.

6.3. **Rotations in dimension 3.** Matrices for rotation about the three coordinate axes have a form related to the 2 dimensional rotation matrices:

Rotation about the x axis

$$\mathrm{R}\left(\mathbf{e}_1,\theta\right)=\mathrm{R}_x(\theta)=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\theta & -\sin\theta\\ 0 & \sin\theta & \cos\theta\end{pmatrix} \tag{3}$$

Rotation about the y axis

$$\mathrm{R}\left(\mathbf{e}_2,\theta\right)=\mathrm{R}_y(\theta)=\begin{pmatrix}\cos\theta & 0 & \sin\theta\\ 0 & 1 & 0\\ -\sin\theta & 0 & \cos\theta\end{pmatrix} \tag{4}$$

Rotation about the z axis

$$\mathrm{R}\left(\mathbf{e}_3,\theta\right)=\mathrm{R}_z(\theta)=\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{5}$$

The vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ along the x, y and z axes are sometimes also denoted $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ respectively.

Within each of these three types, or subgroups, computations are much the same as in two dimensions. The rotations $\mathrm{R}\left(\mathbf{e}_1,\theta\right)$, for example, are exactly the ones that leave the vector $\mathbf{e}_1$ fixed and can be identified with rotation in the yz plane. The rotations $\mathrm{R}\left(\mathbf{e}_1,\theta\right)$ commute,

$$\begin{aligned}\mathrm{R}\left(\mathbf{e}_1,\theta\right)\mathrm{R}\left(\mathbf{e}_1,\phi\right)&=\mathrm{R}\left(\mathbf{e}_1,\theta+\phi\right)\\ &=\mathrm{R}\left(\mathbf{e}_1,\phi+\theta\right)\\ &=\mathrm{R}\left(\mathbf{e}_1,\phi\right)\mathrm{R}\left(\mathbf{e}_1,\theta\right).\end{aligned}$$

The same remarks hold for the subgroups $\mathrm{R}\left(\mathbf{e}_2,\theta\right)$ and $\mathrm{R}\left(\mathbf{e}_3,\theta\right)$. In general, however, rotations in three dimensions do not commute.

Since SO(3) is a group we can get other rotations by multiplying together rotations of the form R_x, R_y, and R_z. It can be shown that any rotation $\mathbf{A}$ can be written as a product of three rotations about the y and z axes,

$$\mathbf{A}=\mathrm{R}_z(\alpha)\mathrm{R}_y(\gamma)\mathrm{R}_z(\delta). \tag{6}$$

The angles α, γ, δ are called *Euler angles* for the rotation $\mathbf{A}$.

6.4. **Rotations and cross products.** We know that rotations are orthogonal transformations distinguished by the fact that they preserve orientation. This is a consequence of the fact that they preserve the vector cross product:

$$\mathbf{A}(\mathbf{v}\times\mathbf{w})=\mathbf{A}\mathbf{v}\times\mathbf{A}\mathbf{w}, \tag{7}$$

for all $\mathbf{A}$ in SO(3) and $\mathbf{v}$ and $\mathbf{w}$ in $\mathbb{R}^3$. So the cross product of rotated vectors is the rotation of the cross product.

Equation (7) follows from the geometric definition of the cross product $\mathbf{v}\times\mathbf{w}$: the cross product $\mathbf{v}\times\mathbf{w}$ is the vector perpendicular to $\mathbf{v}$ and $\mathbf{w}$, determined by the right hand rule, and of length $|\mathbf{v}||\mathbf{w}|\sin\theta$, where θ is the angle between the vectors. All of the terms in this definition are unchanged under rotation since lengths, angles and right handedness are preserved.

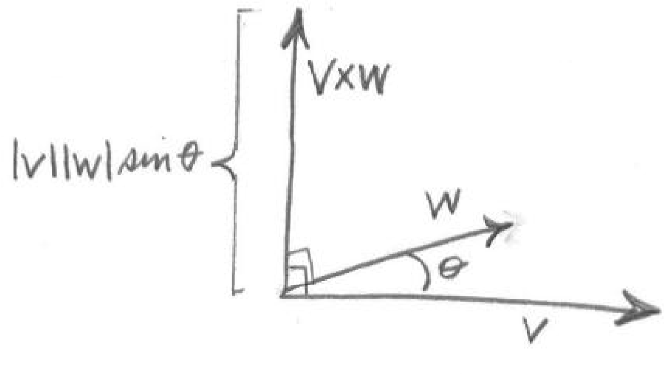

FIGURE 1. The geometric definition of the cross product. The direction of $\mathbf{v} \times \mathbf{w}$ is determined by the right hand rule.

6.5. **Eigenvalues of a rotation.**

6.5.1. *Rotations in complex form.* The rotations around the axes can be written conveniently in complex form. For example, consider rotation an angle θ about the z axis. It can be written simply as

$$(x+iy) \to e^{i\theta}(x+iy) \qquad (8)$$
$$z \to z$$

By writing $\zeta = x + iy$ we can write this as

$$\begin{pmatrix} \zeta \\ z \\ \bar{\zeta} \end{pmatrix} \to \begin{pmatrix} e^{i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{pmatrix} \begin{pmatrix} \zeta \\ z \\ \bar{\zeta} \end{pmatrix} \qquad (9)$$

So using complex vectors gives us a diagonal matrix for this rotation.

Let

$$\mathbf{v} = \frac{1}{2}\left(\mathbf{e}_1 - i\mathbf{e}_2\right). \qquad (10)$$

Since

$$x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3 = \zeta\mathbf{v} + z\mathbf{e}_3 + \bar{\zeta}\bar{\mathbf{v}} \qquad (11)$$

we see that $(\zeta, z, \bar{\zeta})'$ are coordinates of this vector in the frame $(\mathbf{v}, \mathbf{e}_3, \bar{\mathbf{v}})$.

6.5.2. *Eigenvalues.* We will show that the eigenvalues of any rotation are of the form

$$1, e^{i\theta}, e^{-i\theta}$$

for some angle θ. The angle θ is the angle of rotation and the eigenvector corresponding to $e^{i\theta}$ will give the axis.

First we show that *the eigenvalues of an orthogonal matrix have absolute value 1.*

To see this, suppose

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}. \tag{12}$$

then taking the adjoint get

$$\mathbf{v}^*\mathbf{A}^* = \overline{\lambda}\mathbf{v}^*. \tag{13}$$

Since $\mathbf{A}$ is real, $\mathbf{A}^* = \mathbf{A}'$, and multiplying (12) and (13) and using the fact that $\mathbf{A}'\mathbf{A} = \mathbf{I}$ get

$$\mathbf{v}^*\mathbf{v} = |\lambda|^2\mathbf{v}^*\mathbf{v}$$

and hence

$$|\lambda|^2 = 1.$$

If λ is an eigenvalue, so is $\bar{\lambda}$. This follows from (12) by taking the conjugate of both sides and noting that since the entries of $\mathbf{A}$ are real, $\overline{\mathbf{A}} = \mathbf{A}$. If $\mathbf{v}$ is the eigenvector corresponding to λ, then $\bar{\mathbf{v}}$ is the eigenvector corresponding to $\bar{\lambda}$.

From the above discussion and the fact that every complex number of absolute value 1 can be written as $e^{i\theta}$, it follows that the three eigenvalues of an orthogonal matrix A are

$$\pm 1 \qquad \lambda \qquad \bar{\lambda}$$

with

$$\lambda = e^{i\theta} \qquad \bar{\lambda} = e^{-i\theta}.$$

The determinant of $\mathbf{A}$ is the product of the eigenvalues, and for a rotation matrix the determinant is 1. So for a rotation matrix the first eigenvalue above is 1. In what follows denote corresponding eigenvectors by

$$\mathbf{u}, \mathbf{v}, \text{ and } \bar{\mathbf{v}}$$

respectively. The eigenvector $\mathbf{u}$ is real.

If the coordinates of vectors are written in the frame $(\mathbf{v}, \mathbf{u}, \bar{\mathbf{v}})$, then the matrix for the rotation is diagonal as in (9).

6.6. **Axis and angle of rotation.** Intuitively we know that all rotations except for $\mathbf{I}$ have an axis and an angle of rotation. The fact that there is an axis can be seen from the eigenvalues. The eigenvector $\mathbf{u}$ corresponding to the eigenvalue 1 of a rotation matrix gives the axis of rotation. The eigenvector equation (12) shows that this line is left fixed.

The angle of rotation is found from the other two eigenvectors. The argument θ of the eigenvalue $e^{i\theta}$ gives the angle of rotation around the axis. To see this, we need a basic fact about orthogonal matrices:

If $\mathbf{a}$ *and* $\mathbf{b}$ *are eigenvectors of an orthogonal matrix corresponding to distinct eigenvalues then* $\mathbf{a}^*\mathbf{b} = 0$.

This fact is easy to prove. It is left as an exercise to prove it from the definitions of eigenvector and orthogonal. It follows that

$$\mathbf{u}\cdot\mathbf{v} = 0 \qquad \mathbf{u}\cdot\mathbf{v}^* = 0 \qquad \mathbf{v}\cdot\mathbf{v} = 0. \tag{14}$$

Now write

$$\mathbf{v} = \mathbf{v}_1 - i\mathbf{v}_2 \qquad \bar{\mathbf{v}} = \mathbf{v}_1 + i\mathbf{v}_2$$

where $\mathbf{v}_1$ and $\mathbf{v}_2$ are real vectors. It follows from (14) that

$$\mathbf{u}\cdot\mathbf{v}_1 = \mathbf{u}\cdot\mathbf{v}_2 = 0 \tag{15}$$

and so the real vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ are in the plane perpendicular to $\mathbf{u}$. Replacing $\mathbf{u}$ by $-\mathbf{u}$ if necessary we may assume $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{u})$ is a right handed frame. Since

$$\mathbf{v} \to e^{i\theta}\mathbf{v} \tag{16}$$

we see as in the previous section that the rotation $\mathbf{A}$ is an angle θ counterclockwise around $\mathbf{u}$. Write

$$\mathbf{A} = \mathrm{R}\,(\mathbf{u}, \theta)\,. \tag{17}$$

6.7. **Properties of rotations.** A few of the main properties of rotations are summarized here. In what follows, $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ are vectors in $\mathbb{R}^3$, $\mathbf{u} \neq 0$, and $\mathbf{A}$ is a rotation,

$$\mathrm{R}\,(\mathbf{u}, \theta) = \mathrm{R}\,(-\mathbf{u}, -\theta) \tag{18}$$

$$\mathbf{Av} \cdot \mathbf{Aw} = \mathbf{v} \cdot \mathbf{w} \tag{19}$$

$$\mathbf{Av} \times \mathbf{Aw} = \mathbf{A}(\mathbf{v} \times \mathbf{w}) \tag{20}$$

$$\mathbf{u} \cdot (\mathrm{R}\,(\mathbf{u}, \theta)\,\mathbf{v} - \mathbf{v}) = \mathbf{0} \tag{21}$$

$$\mathbf{A}\mathrm{R}\,(\mathbf{u}, \theta)\,\mathbf{A}^{-1} = \mathrm{R}\,(\mathbf{Au}, \theta) \tag{22}$$

If $\mathbf{u}$ is a unit vector,

$$\begin{aligned} &\mathrm{R}\,(\mathbf{u}, \theta)\,\mathbf{v} \\ &= \cos\theta\,(\mathbf{v} - (\mathbf{u}\cdot\mathbf{v})\mathbf{u}) + \sin\theta\,\mathbf{u}\times\mathbf{v} + (\mathbf{u}\cdot\mathbf{v})\mathbf{u} \end{aligned} \tag{23}$$

The identities (19) and (20) were shown above.

Proof of (21). Let $\mathbf{A} = \mathrm{R}\,(\mathbf{u}, \theta)$. Since $\mathbf{Au} = \mathbf{u}$,

$$\mathbf{u} \cdot (\mathbf{Av} - \mathbf{v}) = \mathbf{u} \cdot \mathbf{Av} - \mathbf{u} \cdot \mathbf{v} = \mathbf{Au} \cdot \mathbf{Av} - \mathbf{u} \cdot \mathbf{v} = \mathbf{0}.$$

The last equation follows from (19). □

Proof of (22). The eigenvalues of the matrices on either side of the equation are the same. Note that $\mathbf{Au}$ is left fixed by the matrix on the left side.

□

Proof of (23). Multiplying both sides of the equation by a rotation $\mathbf{A}$ is the same as replacing $\mathbf{u}$ by $\mathbf{Au}$ and $\mathbf{v}$ by $\mathbf{Av}$, so without loss of generality assume $\mathbf{u} = \mathbf{e}_3$. Now check that the equation holds for $\mathbf{v} = \mathbf{e}_1$ and $\mathbf{v} = \mathbf{e}_2$.

The formula can also be seen geometrically. The vector $\mathbf{v}$ is written as the sum of its projection onto $\mathbf{u}$ and onto the plane perpendicular to $\mathbf{u}$,

$$\mathbf{v} = (\mathbf{v} \cdot \mathbf{u})\mathbf{u} + (\mathbf{v} - (\mathbf{u} \cdot \mathbf{v})\mathbf{u}).$$

The projection onto $\mathbf{u}$ is left fixed and the projection onto the plane is rotated an angle θ in the plane. □

Equation (23) gives a way to compute $\mathrm{R}\,(\mathbf{u}, \theta)$ for a unit vector $\mathbf{u}$. If $\mathbf{u} = (a, b, c)'$ write

$$\mathbf{S}_\mathbf{u} = \begin{pmatrix} 0 & -c & b \\ c & 0 & -a \\ -b & a & 0 \end{pmatrix} \tag{24}$$

Note that for any vector $\mathbf{v}$, $\mathbf{Sv} = \mathbf{u} \times \mathbf{v}$. Now (23) shows that

$$\mathrm{R}\,(\mathbf{u}, \theta) = (\cos\theta)\,\mathbf{I} + (1 - \cos\theta)\mathbf{u}'\mathbf{u} + \mathbf{S}_\mathbf{u}$$

6.8. **Shortcuts.** We can find the axis of rotation of $\mathbf{A}$ by finding the eigenvector corresponding to the eigenvalue 1. There is a shortcut for finding the axis if the angle of rotation is not π. The matrix $\mathbf{S} = \mathbf{A} - \mathbf{A}'$ is easily seen to be *skew symmetric*, i. e., $\mathbf{S}' = -\mathbf{S}$. So $\mathbf{S}$ must be of the form (24) If the vector $\mathbf{u} = (a, b, c)'$ is not zero, it is parallel to the axis of rotation of $\mathbf{A}$.

There is also a shortcut for finding the angle θ of rotation. Recall that the trace of a matrix is the sum of the diagonal elements. We have

$$\text{trace}(\mathbf{A}) = 1 + 2\cos\theta$$

so we can solve for $\cos\theta$ from the trace of $\mathbf{A}$. However, we do not know without further investigation if the rotation is an angle of θ clockwise or counterclockwise about $\mathbf{u}$.

See the homework exercise for explanation of why these shortcuts work.

6.9. **Summary.**

(1) A real matrix $\mathbf{A}$ is a rotation matrix if $\mathbf{A}'\mathbf{A} = I$ and $\det \mathbf{A} = 1$.
(2) A rotation matrix preserves the cross product and the dot product.
(3) Every rotation can be written in the form

$$R(\mathbf{u}, \theta) = R(-\mathbf{u}, -\theta)$$

where $\mathbf{u}$ gives the axis direction and θ the angle of rotation.
(4) The eigenvalues of a rotation matrix $\mathbf{A}$ are 1, $e^{i\theta}$ and $e^{-i\theta}$ and
  (a) the angle θ is the angle of rotation
  (b) if $\mathbf{u}$ the eigenvector corresponding to the eigenvalue 1, then $\pm\mathbf{u}$ gives the axis of rotation.
  (c) if $\mathbf{v} = \mathbf{v}_1 - i\mathbf{v}_2$, with $\mathbf{v}_1$ and $\mathbf{v}_2$ real, is an eigenvector corresponding to the eigenvalue $e^{i\theta}$, $e^{i\theta}$ and $(\mathbf{v}_1, \mathbf{v}_2, \mathbf{u})$ is positively oriented then

$$\mathbf{A} = \mathrm{R}\left(\mathbf{u}, \theta\right).$$