Rotation Matrices in two, three and many dimensions

1. Proper and improper rotation matrices in n dimensions

A matrix is a representation of a linear transformation, which can be viewed as a machine that consumes a vector and spits out another vector. A rotation is a transformation with the property that the vector consumed by the machine and the vector spit out by the machine have the same length. That is, physically rotating a vector by an angle θ leaves the length of the vector unchanged. As a matrix equation, if R is a rotation matrix and $\vec{\boldsymbol{v}}$ is a vector, then

$$\vec{\boldsymbol{w}} = R\vec{\boldsymbol{v}}\,, \quad \text{where } \|\vec{\boldsymbol{w}}\| = \|\vec{\boldsymbol{v}}\|. \tag{1}$$

In eq. (1), the length of the vector $\vec{\boldsymbol{v}}$ is denoted by $\|\vec{\boldsymbol{v}}\|$. Note that if $\vec{\boldsymbol{v}}$ is a vector in an n-dimensional space, then in terms of the components of $\vec{\boldsymbol{v}} = (v_1, v_2, \ldots, v_n)$ and $\vec{\boldsymbol{w}} = (w_1, w_2, \ldots, w_n)$, eq. (1) is equivalent to

$$w_i = \sum_{j=1}^{n} R_{ij} v_j\,, \tag{2}$$

where R_{ij} are the matrix elements of the rotation matrix R. In addition, the length of the vector $\vec{\boldsymbol{v}}$ is given by the n-dimensional generalization of the Pythagorean theorem,

$$\|\vec{\boldsymbol{v}}\| = \sqrt{v_1^2 + v_2^2 + \ldots + v_n^2}\,, \tag{3}$$

with a similar formula for the length of $\vec{\boldsymbol{w}}$.

Let us now ask the following question: what is the most general form of the matrix R such that the lengths of the vectors $\vec{\boldsymbol{v}}$ and $\vec{\boldsymbol{w}}$ are equal, as specified in eq. (1)? That is, what is the most general form of R in eq. (2) such that

$$\sum_{i=1}^{n} w_i w_i = \sum_{i=1}^{n} v_i v_i\,, \tag{4}$$

which is the condition that must be satisfied if $\|\vec{\boldsymbol{v}}\| = \|\vec{\boldsymbol{w}}\|$ in light of eq. (3). To answer this question, we insert eq. (2) into the left hand side of eq. (3). Here, we must be careful with indices and write:

$$w_i w_i = \sum_{j=1}^{n} R_{ij} v_j \sum_{k=1}^{n} R_{ik} v_k\,. \tag{5}$$

The second time we write w_i as a sum on the right hand side of eq. (5), one must use a different summation index (e.g., k), since the index j has already been used as a summation index in the first sum. The best way to see this is to take a simple example, say with $i = 1$ and $n = 2$. Then eq. (5) yields

$$w_1^2 = (R_{11}v_1 + R_{12}v_2)(R_{11}v_1 + R_{12}v_2)\,. \tag{6}$$

It would be wrong to write

$$w_i w_i = \sum_{j=1}^{n} R_{ij}v_j R_{ij}v_j\,, \qquad \textit{WRONG!},$$

which in our simple example with $i = 1$ and $n = 2$ would yield $w_1^2 = R_{11}^2 v_1^2 + R_{12}^2 v_2^2$, thereby missing the cross terms that appear when multiplying out the two factors on the right hand side of eq. (6).

Since the sums in eq. (5) consist of a finite number of terms, one can move the summation signs to the left and reorder the terms being multiplied to obtain,

$$w_i w_i = \sum_{j=1}^{n}\sum_{k=1}^{n} R_{ij}R_{ik}v_j v_k\,. \tag{7}$$

Next, we sum over the free index i on both sides of eq. (7) and use eq. (4) to obtain,

$$\sum_{i=1}^{n} w_i w_i = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} R_{ij}R_{ik}v_j v_k = \sum_{i=1}^{n} v_i v_i\,. \tag{8}$$

One can now use the following trick. Recalling the definition of the Kronecker delta symbol,

$$\delta_{jk} = \begin{cases} 1\,, & \text{if } j = k, \\ 0\,, & \text{if } j \neq k, \end{cases} \tag{9}$$

it follows that the right hand side of eq. (8) can be rewritten as

$$\sum_{i=1}^{n} v_i v_i = \sum_{j=1}^{n}\sum_{k=1}^{n} \delta_{jk} v_j v_k\,. \tag{10}$$

As this is one of the crucial steps in the analysis, you should convince yourself that eq. (10) is an identity (e.g., by examining the case of $n = 2$ and writing out the sums explicitly). One can now insert eq. (10) back into eq. (8) to obtain,

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} R_{ij}R_{ik}v_j v_k = \sum_{j=1}^{n}\sum_{k=1}^{n} \delta_{jk} v_j v_k\,. \tag{11}$$

Interchanging the order of summation,

$$\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{i=1}^{n} R_{ij}R_{ik}v_j v_k = \sum_{j=1}^{n}\sum_{k=1}^{n} \delta_{jk} v_j v_k\,. \tag{12}$$

Moving the right hand side above over to the left hand side of eq. (12) yields,

$$\sum_{j=1}^{n}\sum_{k=1}^{n}\left[\left(\sum_{i=1}^{n} R_{ij}R_{ik}\right)-\delta_{jk}\right]v_j v_k = 0\,. \tag{13}$$

Let us denote the expression inside the square brackets as,

$$A_{jk} \equiv \left(\sum_{i=1}^{n} R_{ij}R_{ik}\right)-\delta_{jk}\,, \tag{14}$$

in which case, eq. (13) is equivalent to

$$\sum_{j=1}^{n}\sum_{k=1}^{n} A_{jk}v_j v_k = 0\,. \tag{15}$$

In the above analysis, I never specified a specific value for the v_j. In other words, if one were to rotate any vector $\vec{\boldsymbol{v}}$, the end result would still be eq. (15). This observation implies that eq. (15) must be true for any choice of the v_j. Consequently, it must be true that $A_{jk}=0$ for all $j,k=1,2,\ldots,n$.[1] Inserting $A_{jk}=0$ into the left hand side of eq. (14) yields out final result,

$$\boxed{\sum_{i=1}^{n} R_{ij}R_{ik} = \delta_{jk}\,.} \tag{16}$$

To interpret eq. (16), I remind you that the jk element of the product of two $n\times n$ matrices is given by the formula [cf. eq. (9.3) in Chapter 3, p. 138 of Boas],

$$(BC)_{jk} = \sum_{i=1}^{n} B_{ji}C_{ik}\,. \tag{17}$$

Inserting $B=R^{\mathsf{T}}$ and $C=R$ in eq. (17) and using eq. (16) then yields the matrix equation $R^{\mathsf{T}}R=\mathbf{I}$. In obtaining this result, we noted that the matrix elements of the identity matrix are $\mathbf{I}_{ij}=\delta_{ij}$, and the transpose of a matrix interchanges the rows and columns, so that $(R^{\mathsf{T}})_{ji}=R_{ij}$. In conclusion, eq. (16) in matrix form is equivalent to the statement that

$$R^{\mathsf{T}}R=\mathbf{I}\,. \tag{18}$$

A matrix R that satisfies eq. (18) is called an *orthogonal matrix*. Multiplying both sides of eq. (18) on the right by R^{-1} and using $RR^{-1}=\mathbf{I}$ yields,

$$R^{\mathsf{T}} = R^{-1}\,. \tag{19}$$

[1] For example, choose $\vec{\boldsymbol{v}}=(1,0,0,\ldots,0)$ and insert this choice in eq. (15) to obtain $A_{11}=0$. Now keep on choosing vectors with different components, and eventually you will see that $A_{jk}=0$ for all $j,k=1,2,\ldots,n$.

which can also be used as the definition of an orthogonal matrix. Finally, multiplying both sides of eq. (19) on the left by R and again using $RR^{-1} = \mathbf{I}$ yields,

$$RR^{\mathsf{T}} = \mathbf{I}\,. \tag{20}$$

Hence, orthogonal matrices are matrices that satisfy $R^{-1} = R^{\mathsf{T}}$, or equivalently satisfy,

$$R^{\mathsf{T}}R = RR^{\mathsf{T}} = \mathbf{I}\,. \tag{21}$$

We conclude that rotation matrices must be real orthogonal matrices.

Next, consider the following question. Can any real $n \times n$ orthogonal matrix be identified as some rotation matrix in n-dimensional space [which is the converse of statement following eq. (21)]? To gain some insight, let us take the determinant of both sides of eq. (18). Recall that $\det \mathbf{I} = 1$ and that for any $n \times n$ matrices B and C, we have $\det(BC) = (\det B)(\det C)$. Finally, for any matrix B, we have $\det(B^{\mathsf{T}}) = \det B$. Making use of these properties, eq. (18) yields,

$$\det(R^{\mathsf{T}}R) = (\det R^{\mathsf{T}})(\det R) = (\det R)^2 = \det \mathbf{I} = 1\,. \tag{22}$$

It then follows that[2]

$$\det R = \pm 1\,. \tag{23}$$

That is, some real orthogonal matrices have determinant equal to 1, whereas other real orthogonal matrices have determinant equal to -1. In these notes, I shall explore the explicit forms for rotation matrices in 2 and 3 dimensions. Extending those results to n dimensions, one can show that any real $n \times n$ orthogonal matrix with determinant equal to 1 can be identified as some rotation matrix in n dimensions. A real orthogonal matrix with determinant equal to -1 can be identified as a product of a rotation and a reflection.

The above observation leads to the following nomenclature. A real orthogonal matrix R with $\det R = 1$ provides a matrix representation of a *proper rotation*. The most general rotation matrix R represents a counterclockwise rotation by an angle θ about a fixed axis that is parallel to the unit vector $\hat{\boldsymbol{n}}$.[3] The rotation matrix operates on vectors to produce rotated vectors, while the coordinate axes are held fixed. In typical parlance, a rotation refers to a proper rotation. Thus, in the following sections of these notes we will often omit the adjective *proper* when referring to a proper rotation.

A real orthogonal matrix $\overline{R}$ with $\det \overline{R} = -1$ provides a matrix representation of an *improper rotation*.[4] To perform an improper rotation requires mirrors. That is, the most general improper rotation matrix is a product of a proper rotation by an angle θ about some axis $\hat{\boldsymbol{n}}$ and a mirror reflection through a plane that passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$.

[2]Note that eq. (23) implies that $\det R \neq 0$. This result implies that the inverse of a rotation matrix, R^{-1} always exist. We implicitly used this fact to go from eq. (18) to eq. (19), so this step is now justified.

[3]The corresponding inverse matrix R^{-1} represents a clockwise rotation by an angle θ about a fixed axis that is parallel to the unit vector $\hat{\boldsymbol{n}}$. With this observation, you can quickly check that $RR^{-1} = \mathbf{I}$, as expected.

[4]To distinguish matrices representing improper rotations from those of proper rotations, we shall employ the notation $\overline{R}$ to denote an improper rotation matrix.

Finally, it is instructive to consider the following question: how many real independent parameters (which we shall denote by N below) describe a real orthogonal $n \times n$ matrix? To answer this question, we start with eq. (16). A general real $n \times n$ matrix possesses n^2 parameters (corresponding to its n^2 matrix elements). But, eq. (16) imposes constraints on these n^2 parameters. Consider first the case of $j = k$. Then eq. (16) reduces to,

$$\sum_{i=1}^{n} R_{ij} R_{ij} = 1 \,, \quad \text{for } j = 1, 2, \ldots, n. \tag{24}$$

That is, eq. (24) constitutes n independent constraint equations. Next, we consider the case of $j \neq k$, Then eq. (16) reduces to

$$\sum_{i=1}^{n} R_{ij} R_{ik} = 0 \,, \quad \text{for } j < k \text{ with } j, k = 1, 2, \ldots, n. \tag{25}$$

Note that one only has to consider $j < k$, since the equations for $j > k$ do not give any further independent constraints.[5] To determine the number of independent constraint equations that are contained in eq. (25), one must simply count up the number of possible choices of $j < k$, with $j, k = 1, 2, \ldots, n$. The number of pairs $\{j, k\}$ with $j \neq k$ is equal to $n^2 - n$ (after subtracting off the n pairs with $j = k$). Of these $n^2 - n$ pairs, half of them have $j < k$ and half of them have $j > k$. Hence, eq. (25) constitutes $\frac{1}{2}n(n-1)$ constraint equations.

One can conclude that the number of constraint equations imposed by eq. (16) on the n^2 parameters of the matrix R is

$$n + \tfrac{1}{2}n(n-1) = \tfrac{1}{2}n(n+1) \,. \tag{26}$$

Subtracting this value from the n^2 parameters of a real $n \times n$ matrix leaves us with

$$N \equiv n^2 - \tfrac{1}{2}n(n+1) = \tfrac{1}{2}n(n-1) \tag{27}$$

independent (unconstrained) parameters. That is, a real orthogonal $n \times n$ matrix depends on $N = \frac{1}{2}n(n-1)$ independent parameters.

Consider how this works for $n = 2$ and $n = 3$. In the case of $n = 2$, eq. (27) yields $N = 1$. This is not surprising, since the most general two-dimensional rotation consists of a rotation by an angle θ in the plane. Thus, we identify θ as the one independent parameter. In the case of $n = 3$, eq. (27) yields $N = 3$. This is again not a surprise. Indeed, as noted above, the most general rotation in three dimensions consists of a counterclockwise rotation by an angle θ about a fixed axis that lies along the unit vector $\hat{\boldsymbol{n}}$. The direction of $\hat{\boldsymbol{n}}$ is fixed by two angles $\theta_{\boldsymbol{n}}$ and $\phi_{\boldsymbol{n}}$, corresponding to its polar angle and azimuthal angle with respect to a fixed z-axis. Thus, the three angles, $\{\theta, \theta_{\boldsymbol{n}}, \phi_{\boldsymbol{n}}\}$ constitute the three independent parameters that describe an arbitrary three-dimensional proper rotation.

[5] To verify this claim, rewrite eq. (25) as $\sum_{i=1}^{n} R_{ik} R_{ij} = 0$ for $j > k$ and notice that this is precisely the same form as eq. (25) in the case of $k < j$.

2. Properties of 2×2 proper and improper rotation matrices

In the case of $n=2$. it is easy to work out the form of the most general real orthogonal matrix. Taking $R=\left(\begin{smallmatrix} a & b\\ c & d\end{smallmatrix}\right)$, and imposing $RR^{\mathsf{T}}=\mathbf{I}$ [cf. eq. (19)],

$$\begin{pmatrix} a & b\\ c & d\end{pmatrix}\begin{pmatrix} a & c\\ b & d\end{pmatrix}=\begin{pmatrix} 1 & 0\\ 0 & 1\end{pmatrix}\,. \tag{28}$$

Performing the matrix multiplication, we end up with,

$$\begin{pmatrix} a^2+b^2 & ac+bd\\ ac+bd & c^2+d^2\end{pmatrix}=\begin{pmatrix} 1 & 0\\ 0 & 1\end{pmatrix}\,. \tag{29}$$

Thus, we obtain three constraint equations, as expected from eq. (26),

$$a^2+b^2=1\,, \tag{30}$$
$$c^2+d^2=1\,, \tag{31}$$
$$ac+bd=0\,. \tag{32}$$

We now consider separately the cases of proper and improper rotations. In the case of proper rotations, we add a fourth equation to eqs. (30)–(32),

$$\det R=ad-bc=1\,. \tag{33}$$

Suppose that $b\neq 0$ and $c\neq 0$.[6] From eq. (32), it follows that $d=-ac/b$. Substituting this into eq. (33) yields,

$$a^2+b^2=-\frac{b}{c}\,. \tag{34}$$

Combining eqs. (30) and (34), we conclude that $b=-c$. Plugging this result back into eq. (32) yields $a=d$. With these results, eq. (31) is automatically satisfied in light of eq. (30). Hence, the most general 2×2 real orthogonal matrix with determinant equal to 1 is given by,[7]

$$R=\begin{pmatrix} a & b\\ -b & a\end{pmatrix}\,,\qquad\text{with } a^2+b^2=1 \text{ and } |a|\leq 1,\ |b|\leq 1. \tag{35}$$

Without loss of generality, we can set $a=\cos\theta$ and $b=\pm\sqrt{1-a^2}=\pm\sin\theta$, since $\cos\theta$ and $\sin\theta$ satisfy the same properties as a and b, namely, $\sin^2\theta+\cos^2\theta=1$ and $|\sin\theta|\leq 1$, $|\cos\theta|\leq 1$ for $0\leq\theta<2\pi$. Indeed, the rotation matrix,

$$R=\begin{pmatrix} \cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\,,\qquad\text{where } 0\leq\theta<2\pi\,, \tag{36}$$

represents a proper counterclockwise rotation by an angle θ in the plane, as discussed in class (see p. 127 of Boas).

[6] The case of $b=0$ or $c=0$ can be treated separately. This is left as an exercise for the student. These special cases will not change the general result obtained in eq. (35).

[7] Note that $|a|\leq 1$ and $|b|\leq 1$ is actually a consequence of $a^2+b^2=1$.

In the case of improper rotations, we start with $\overline{R} = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ and impose $\overline{R}\,\overline{R}^{\mathsf{T}} = \mathbf{I}$, which again yields eqs. (28)–(32). We then add a fourth equation to eqs. (30)–(32),

$$\det \overline{R} = ad - bc = -1\,. \tag{37}$$

Suppose that $b \neq 0$ and $c \neq 0$ (with the case of $b = 0$ or $c = 0$ again left as an exercise for the student). From eq. (32), it follows that $d = -ac/b$. Substituting this into eq. (33) yields,

$$a^2 + b^2 = \frac{b}{c}\,. \tag{38}$$

Combining eqs. (30) and (34), we conclude that $b = c$. Plugging this result back into eq. (32) yields $a = -d$. With these results, eq. (31) is automatically satisfied in light of eq. (30). Hence, the most general 2×2 real orthogonal matrix with determinant equal to -1 is given by,

$$\overline{R} = \begin{pmatrix} a & b \\ b & -a \end{pmatrix}\,, \quad \text{with } a^2 + b^2 = 1 \text{ and } |a| \leq 1,\ |b| \leq 1. \tag{39}$$

We can again set $a = \cos\theta$ and $b = \pm\sqrt{1 - a^2} = \pm\sin\theta$. Thus, an example of an improper rotation matrix is,

$$\overline{R} = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\,, \quad \text{where } 0 \leq \theta < 2\pi\,. \tag{40}$$

This matrix satisfies the property, $\overline{R}^{\,2} = \mathbf{I}$.

Note that we can express R given in eq. (40) as the product of a proper rotation and a reflection,

$$\overline{R} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,. \tag{41}$$

In particular, looking at the effect of $\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ on the vector $\vec{\boldsymbol{v}} = (x, y)$,

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ -y \end{pmatrix}\,,$$

it follows that the effect of $\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is to reflect a two dimensional vector through the x-axis. Note that our statement that real orthogonal 2×2 matrices depend on one real parameter applies both to proper and improper rotations, since the presence or absence of a reflection does not alter the parameter count.

However, $\overline{R}^{\,2} = \mathbf{I}$ suggests that the action of $\overline{R}$ consists of a pure reflection through a fixed line that lies in the x–y plane, since two successive applications of such a reflection is equivalent to the identity transformation. Indeed, in the class handout entitled *Eigenvalues and eigenvectors of rotation matrices*, it is shown that the action of $\overline{R}$ corresponds to a reflection through a straight line of slope $\tan\!\left(\tfrac{1}{2}\theta\right)$ that passes through the origin. This result can be verified by a geometric argument, which is left as an exercise for the reader.

In conclusion, an arbitrary real orthogonal 2×2 matrix with determinant -1 corresponds to a pure reflection through a fixed line that passes through the origin.

3. Properties of the 3×3 proper rotation matrix

It becomes quickly evident that the methods used in the previous section become much less practical for $n = 3$. In this section I shall present the explicit form of the 3×3 proper rotation matrix along with its most important properties. A derivation of the rotation matrix is given in an Appendix to these notes.

As previously noted, the most general three-dimensional rotation, which we henceforth denote by $R(\hat{\boldsymbol{n}}, \theta)$, can be specified by an axis of rotation pointing in the direction of the unit vector $\hat{\boldsymbol{n}}$, and a rotation angle θ. Conventionally, a positive rotation angle corresponds to a counterclockwise rotation. The direction of the axis is determined by the right hand rule. Namely, curl the fingers of your right hand around the axis of rotation, where your fingers point in the θ direction. Then, your thumb points perpendicular to the plane of rotation in the direction of $\hat{\boldsymbol{n}}$. In general, rotation matrices do not commute under multiplication. However, if both rotations are taken with respect to the *same* fixed axis, then

$$R(\hat{\boldsymbol{n}}, \theta_1) R(\hat{\boldsymbol{n}}, \theta_2) = R(\hat{\boldsymbol{n}}, \theta_1 + \theta_2) \,. \tag{42}$$

Simple geometric considerations will convince you that the following relations are satisfied:

$$R(\hat{\boldsymbol{n}}, \theta + 2\pi k) = R(\hat{\boldsymbol{n}}, \theta) \,, \qquad k = 0, \pm 1 \pm 2 \ldots \,, \tag{43}$$

$$[R(\hat{\boldsymbol{n}}, \theta)]^{-1} = R(\hat{\boldsymbol{n}}, -\theta) = R(-\hat{\boldsymbol{n}}, \theta) \,. \tag{44}$$

Combining these two results, it follows that

$$R(\hat{\boldsymbol{n}}, 2\pi - \theta) = R(-\hat{\boldsymbol{n}}, \theta) \,, \tag{45}$$

which implies that any three-dimensional rotation can be described by a counterclockwise rotation by an angle θ about an arbitrary axis $\hat{\boldsymbol{n}}$, where $0 \leq \theta \leq \pi$.[8] However, if we substitute $\theta = \pi$ in eq. (45), we conclude that

$$R(\hat{\boldsymbol{n}}, \pi) = R(-\hat{\boldsymbol{n}}, \pi) \,, \tag{46}$$

which means that for the special case of $\theta = \pi$, $R(\hat{\boldsymbol{n}}, \pi)$ and $R(-\hat{\boldsymbol{n}}, \pi)$ represent the *same* rotation. In particular, note that

$$[R(\hat{\boldsymbol{n}}, \pi)]^2 = \mathbf{I} \,. \tag{47}$$

Indeed for any choice of $\hat{\boldsymbol{n}}$, the $R(\hat{\boldsymbol{n}}, \pi)$ are the only non-trivial rotation matrices whose square is equal to the identity matrix. Finally, if $\theta = 0$ then $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$ is the identity matrix (sometimes called the trivial rotation), independently of the direction of $\hat{\boldsymbol{n}}$.

[8] There is an alternative convention for the range of possible angles θ and rotation axes $\hat{\boldsymbol{n}}$. We say that $\hat{\boldsymbol{n}} = (n_1, n_2, n_3) > 0$ if the first nonzero component of $\hat{\boldsymbol{n}}$ is positive. That is $n_3 > 0$ if $n_1 = n_2 = 0$, $n_2 > 0$ if $n_1 = 0$, and $n_1 > 0$ otherwise. Then, all possible rotation matrices $R(\hat{\boldsymbol{n}}, \theta)$ correspond to $\hat{\boldsymbol{n}} > 0$ and $0 \leq \theta < 2\pi$. However, we will not employ this convention in these notes.

We now present an explicit form for $R(\hat{\boldsymbol{n}},\theta)$. Since $R(\hat{\boldsymbol{n}},\theta)$ describes a rotation by an angle θ about an axis $\hat{\boldsymbol{n}}$, the formula for $R(\hat{\boldsymbol{n}},\theta)$ will depend on the angle θ and on the coordinates of $\hat{\boldsymbol{n}} = (n_1\,,\,n_2\,,\,n_3)$ with respect to a fixed Cartesian coordinate system. Note that since $\hat{\boldsymbol{n}}$ is a unit vector, it follows that,

$$n_1^2 + n_2^2 + n_3^2 = 1\,. \tag{48}$$

We can also express $\hat{\boldsymbol{n}}$ in terms of its polar and azimuthal angles ($\theta_{\boldsymbol{n}}$ and $\phi_{\boldsymbol{n}}$, respectively) with respect to a fixed z-axis. In particular,

$$n_1 = \sin\theta_{\boldsymbol{n}}\cos\phi_{\boldsymbol{n}}\,, \tag{49}$$

$$n_2 = \sin\theta_{\boldsymbol{n}}\sin\phi_{\boldsymbol{n}}\,, \tag{50}$$

$$n_3 = \cos\theta_{\boldsymbol{n}}\,. \tag{51}$$

One can check that eq. (48) is indeed satisfied. Thus, $\hat{\boldsymbol{n}}$ depends on two independent parameters, $\theta_{\boldsymbol{n}}$ and $\phi_{\boldsymbol{n}}$, which together with the rotation angle θ constitute the three independent parameters that describe a three dimensional rotation.

The explicit formula for the real orthogonal 3×3 matrix $R(\hat{\boldsymbol{n}},\theta)$ with determinant equal to 1 is given by,

$$\boxed{R(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} \cos\theta + n_1^2(1-\cos\theta) & n_1n_2(1-\cos\theta) - n_3\sin\theta & n_1n_3(1-\cos\theta) + n_2\sin\theta \\ n_1n_2(1-\cos\theta) + n_3\sin\theta & \cos\theta + n_2^2(1-\cos\theta) & n_2n_3(1-\cos\theta) - n_1\sin\theta \\ n_1n_3(1-\cos\theta) - n_2\sin\theta & n_2n_3(1-\cos\theta) + n_1\sin\theta & \cos\theta + n_3^2(1-\cos\theta) \end{pmatrix}} \tag{52}$$

One can easily check that eqs. (43) and (44) are satisfied. In particular, as indicated by eq. (45), the rotations $R(\hat{\boldsymbol{n}},\pi)$ and $R(-\hat{\boldsymbol{n}},\pi)$ represent the same rotation,

$$R_{ij}(\hat{\boldsymbol{n}},\pi) = \begin{pmatrix} 2n_1^2 - 1 & 2n_1n_2 & 2n_1n_3 \\ 2n_1n_2 & 2n_2^2 - 1 & 2n_2n_3 \\ 2n_1n_3 & 2n_2n_3 & 2n_3^2 - 1 \end{pmatrix} = 2n_in_j - \delta_{ij}\,, \tag{53}$$

where the Kronecker delta symbol was introduced in eq. (9). Finally, as expected, $R_{ij}(\hat{\boldsymbol{n}},0) = \delta_{ij}$, independently of the direction of $\hat{\boldsymbol{n}}$. I leave it as an exercise to the student to verify explicitly that $R = R(\hat{\boldsymbol{n}},\theta)$ given in eq. (52) satisfies the conditions $RR^{\mathsf{T}} = \mathbf{I}$ and $\det R = +1$.

Although eq. (52) looks complicated, one can present an elegant expression for the matrix elements of $R(\hat{\boldsymbol{n}},\theta)$, denoted below by R_{ij}. Indeed, it is not difficult to check that the following expression for R_{ij} is equivalent to the matrix elements of $R(\hat{\boldsymbol{n}},\theta)$ exhibited in eq. (52),

$$\boxed{R_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} + (1-\cos\theta)n_in_j - \sin\theta\sum_{k=1}^{3}\epsilon_{ijk}n_k} \tag{54}$$

where ϵ_{ijk} is the Levi-Civita epsilon symbol, which is defined as follows,

$$\epsilon_{ijk} = \begin{cases} +1\,, & \text{if } \{i,j,k\} \text{ is an even permutation of } \{1,2,3\}, \\ -1\,, & \text{if } \{i,j,k\} \text{ is an odd permutation of } \{1,2,3\}, \\ 0\,, & \text{if not all the integers 1,2,3 are distinct.} \end{cases} \tag{55}$$

Note that ϵ_{ijk} is the $n = 3$ version of the Levi-Civita symbol introduced in the class handout entitled *Determinant and the Adjugate*.

Eq. (54) is called the *Rodriguez formula* for the 3×3 rotation matrix $R(\hat{\boldsymbol{n}}, \theta)$. One possible derivation of this formula is provided in Appendix A.

It is instructive to check special cases of eq. (52). For example, suppose we choose $\hat{\boldsymbol{n}} = \boldsymbol{k}$ corresponding to a rotation axis that points along the positive z-direction. In this case, $n_1 = n_2 = 0$ and $n_3 = 1$, and eq. (52) yields

$$R(\boldsymbol{k}, \theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{56}$$

which reproduces eq. (7.18) of Chapter 3 on p. 129 of Boas. Of course, eq. (56) is the expected result given the form of the two-dimensional rotation matrix given in eq. (36).

Likewise, one can choose either $\hat{\boldsymbol{n}} = \boldsymbol{i}$ or $\hat{\boldsymbol{n}} = \boldsymbol{j}$ corresponding to rotation axes that point along the positive x-direction (i.e., $n_2 = n_3 = 0$ and $n_1 = 1$) or along the positive y-direction (i.e., $n_1 = n_3 = 0$ and $n_2 = 1$), respectively. In theses cases, eq. (52) yields,

$$R(\boldsymbol{i}, \theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \tag{57}$$

$$R(\boldsymbol{j}, \theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}. \tag{58}$$

Note that eq. (58) reproduces eq. (7.20) of Chapter 3 on p. 129 of Boas.

4. Properties of the 3 × 3 improper rotation matrix

An improper rotation matrix is an orthogonal matrix, $\overline{R}$, such that $\det \overline{R} = -1$. The most general three-dimensional improper rotation, denoted by $\overline{R}(\hat{\boldsymbol{n}}, \theta)$, consists of a product of a proper rotation matrix, $R(\hat{\boldsymbol{n}}, \theta)$, and a mirror reflection through a plane normal to the unit vector $\hat{\boldsymbol{n}}$, which we denote by $\overline{R}(\hat{\boldsymbol{n}})$. In particular, the reflection plane passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. In equations,

$$\overline{R}(\hat{\boldsymbol{n}}, \theta) \equiv R(\hat{\boldsymbol{n}}, \theta)\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}}, \theta)\,. \tag{59}$$

Note that the improper rotation defined in eq. (59) does not depend on the order in which the proper rotation and reflection are applied. The matrix $\overline{R}(\hat{\boldsymbol{n}})$ is called a *reflection matrix*, since it is a representation of a mirror reflection through a fixed plane. In particular,

$$\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(-\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}}, 0)\,, \tag{60}$$

after using $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$. Thus, the overall sign of $\hat{\boldsymbol{n}}$ for a reflection matrix has no physical meaning. Note that all reflection matrices are orthogonal matrices with $\det \overline{R}(\hat{\boldsymbol{n}}) = -1$, with the property that:

$$[\overline{R}(\hat{\boldsymbol{n}})]^2 = \mathbf{I}\,, \tag{61}$$

or equivalently,

$$[\overline{R}(\hat{\boldsymbol{n}})]^{-1} = \overline{R}(\hat{\boldsymbol{n}})\,. \tag{62}$$

In general, the product of a two proper and/or improper rotation matrices is not commutative. However, if $\hat{\boldsymbol{n}}$ is the same for both matrices, then eq. (42) implies that:[9]

$$R(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2) = \overline{R}(\hat{\boldsymbol{n}}, \theta_1)R(\hat{\boldsymbol{n}}, \theta_2) = \overline{R}(\hat{\boldsymbol{n}}, \theta_1 + \theta_2)\,, \tag{63}$$

$$\overline{R}(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2) = \overline{R}(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2) = R(\hat{\boldsymbol{n}}, \theta_1 + \theta_2)\,, \tag{64}$$

after making use of eqs. (59) and (61).

The properties of the improper rotation matrices mirror those of the proper rotation matrices given in eqs. (43)–(47). Indeed the properties of the latter combined with eqs. (60) and (62) yield:

$$\overline{R}(\hat{\boldsymbol{n}}, \theta + 2\pi k) = \overline{R}(\hat{\boldsymbol{n}}, \theta)\,, \qquad k = 0, \pm 1\, \pm 2\, \ldots\,, \tag{65}$$

$$[\overline{R}(\hat{\boldsymbol{n}}, \theta)]^{-1} = \overline{R}(\hat{\boldsymbol{n}}, -\theta) = \overline{R}(-\hat{\boldsymbol{n}}, \theta)\,. \tag{66}$$

Combining these two results, it follows that

$$\overline{R}(\hat{\boldsymbol{n}}, 2\pi - \theta) = \overline{R}(-\hat{\boldsymbol{n}}, \theta)\,. \tag{67}$$

We shall adopt the convention (employed in Section 2) in which the angle θ is defined to lie in the interval $0 \leq \theta \leq \pi$. In this convention, the overall sign of $\hat{\boldsymbol{n}}$ is meaningful when $0 < \theta < \pi$. In contrast, for $\theta = \pi$, eq. (67) implies that $\overline{R}(\hat{\boldsymbol{n}}, \pi) = \overline{R}(-\hat{\boldsymbol{n}}, \pi)$.

The matrix $\overline{R}(\hat{\boldsymbol{n}}, \pi)$ is special. Geometric considerations will convince you that

$$\overline{R}(\hat{\boldsymbol{n}}, \pi) = R(\hat{\boldsymbol{n}}, \pi)\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}}, \pi) = -\mathbf{I}\,. \tag{68}$$

That is, $\overline{R}(\hat{\boldsymbol{n}}, \pi)$ represents an *inversion*, which is a linear operator that transforms all vectors $\vec{\boldsymbol{x}} \to -\vec{\boldsymbol{x}}$. In particular, $\overline{R}(\hat{\boldsymbol{n}}, \pi)$ is *independent* of the unit vector $\hat{\boldsymbol{n}}$. Eq. (68)

[9]Since $\det[R(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2)] = \det R(\hat{\boldsymbol{n}}, \theta_1) \det \overline{R}(\hat{\boldsymbol{n}}, \theta_2) = -1$, it follows that $R(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2)$ must be an improper rotation matrix. Likewise, $\overline{R}(\hat{\boldsymbol{n}}, \theta_1)\overline{R}(\hat{\boldsymbol{n}}, \theta_2)$ must be a proper rotation matrix. Eqs. (63) and (64) are consistent with these expectations.

is equivalent to the statement that an inversion is equivalent to a mirror reflection through a plane that passes through the origin and is perpendicular to an arbitrary unit vector $\hat{\boldsymbol{n}}$, followed by a proper rotation of 180° around the axis $\hat{\boldsymbol{n}}$. Sometimes, $\overline{R}(\hat{\boldsymbol{n}},\pi)$ is called a point reflection through the origin (to distinguish it from a reflection through a plane). Just like a reflection matrix, the inversion matrix satisfies

$$[\overline{R}(\hat{\boldsymbol{n}},\pi)]^2 = \mathbf{I}\,. \tag{69}$$

In general, any improper 3×3 rotation matrix $\overline{R}$ with the property that $\overline{R}^2=\mathbf{I}$ is a representation of either an inversion or a reflection through a plane that passes through the origin.

Given any proper 3×3 rotation matrix $R(\hat{\boldsymbol{n}},\theta)$, the matrix $-R(\hat{\boldsymbol{n}},\theta)$ has determinant equal to -1 and therefore represents some improper rotation which can be determined as follows:

$$-R(\hat{\boldsymbol{n}},\theta) = R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}},\pi) = \overline{R}(\hat{\boldsymbol{n}},\theta+\pi) = \overline{R}(-\hat{\boldsymbol{n}},\pi-\theta)\,, \tag{70}$$

after employing eqs. (68), (63) and (67). Two noteworthy consequences of eq. (70) are:

$$\overline{R}(-\hat{\boldsymbol{n}},\tfrac{1}{2}\pi) = -R(\hat{\boldsymbol{n}},\tfrac{1}{2}\pi)\,, \tag{71}$$

$$\overline{R}(\hat{\boldsymbol{n}}) \equiv \overline{R}(\hat{\boldsymbol{n}},0) = -R(\hat{\boldsymbol{n}},\pi)\,, \tag{72}$$

where we have used eq. (46) in obtaining the second equation above.

We now present an explicit formula for the real orthogonal 3×3 matrix $\overline{R}(\hat{\boldsymbol{n}},\theta)$ with determinant equal to -1,

$$\boxed{\overline{R}(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} \cos\theta - n_1^2(1+\cos\theta) & -n_1n_2(1+\cos\theta)-n_3\sin\theta & -n_1n_3(1+\cos\theta)+n_2\sin\theta \\ -n_1n_2(1+\cos\theta)+n_3\sin\theta & \cos\theta-n_2^2(1+\cos\theta) & -n_2n_3(1+\cos\theta)-n_1\sin\theta \\ -n_1n_3(1+\cos\theta)-n_2\sin\theta & -n_2n_3(1+\cos\theta)+n_1\sin\theta & \cos\theta-n_3^2(1+\cos\theta) \end{pmatrix}} \tag{73}$$

One can easily check that eqs. (65) and (66) are satisfied. In particular, as indicated by eq. (60), the improper rotations $\overline{R}(\hat{\boldsymbol{n}},0)$ and $\overline{R}(-\hat{\boldsymbol{n}},0)$ represent the same reflection matrix,[10]

$$\overline{R}_{ij}(\hat{\boldsymbol{n}},0) \equiv \overline{R}_{ij}(\hat{\boldsymbol{n}}) = \begin{pmatrix} 1-2n_1^2 & -2n_1n_2 & -2n_1n_3 \\ -2n_1n_2 & 1-2n_2^2 & -2n_2n_3 \\ -2n_1n_3 & -2n_2n_3 & 1-2n_3^2 \end{pmatrix} = \delta_{ij}-2n_in_j\,. \tag{74}$$

Finally, as expected,

$$\overline{R}_{ij}(\hat{\boldsymbol{n}},\pi) = -\delta_{ij}\,,$$

independently of the direction of $\hat{\boldsymbol{n}}$. I leave it as an exercise to the student to verify explicitly that $\overline{R}=\overline{R}(\hat{\boldsymbol{n}},\theta)$ given in eq. (73) satisfies the conditions $\overline{R}\,\overline{R}^{\mathsf{T}}=\mathbf{I}$ and $\det\overline{R}=-1$.

[10]Indeed, eqs. (53) and (74) are consistent with eq. (72) as expected.

As in the case of eq. (52), one can provide an elegant expression for the matrix elements of $\overline{R}(\hat{\boldsymbol{n}},\theta)$, denoted below by $\overline{R}_{ij}$. Indeed, it is not difficult to check that the following expression for $\overline{R}_{ij}$ is equivalent to the matrix elements of $\overline{R}(\hat{\boldsymbol{n}},\theta)$ exhibited in eq. (73),

$$\boxed{\overline{R}_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} - (1+\cos\theta)n_i n_j - \sin\theta\sum_{k=1}^{3}\epsilon_{ijk}n_k} \tag{75}$$

which is the analog of the Rodriguez formula given in eq. (54).

Note that our statement that real orthogonal 3×3 matrices depend on three real parameters (θ, $\theta_{\boldsymbol{n}}$, $\phi_{\boldsymbol{n}}$) applies both to proper and improper rotations, since the presence or absence of a reflection does not alter the parameter count.

5. Determining the reflection plane of an improper rotation

A general three-dimensional improper rotation matrix, $\overline{R}(\hat{\boldsymbol{n}},\theta) = R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}})$, is the product of a proper rotation and a reflection. The reflection $\overline{R}(\hat{\boldsymbol{n}})$ corresponds to a mirror reflection through a plane perpendicular to $\hat{\boldsymbol{n}}$ that passes through the origin, and $R(\hat{\boldsymbol{n}},\theta)$ represents a counterclockwise rotation by an angle θ with respect to the rotation axis $\hat{\boldsymbol{n}}$. One can easily identify the equation for the reflection plane, which passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. The unit normal to the reflection plane, $\hat{\boldsymbol{n}} = n_1\boldsymbol{i} + n_2\boldsymbol{j} + n_2\boldsymbol{k} = (n_1, n_2, n_3)$, is a vector perpendicular to the reflection plane that passes through the origin, i.e. the point $(x_0, y_0, z_0) = (0,0,0)$. Any vector $\vec{\boldsymbol{v}} = (x,y,z)$ that lies in the reflection plane is perpendicular to $\hat{\boldsymbol{n}}$ and thus satisfies $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{v}} = n_1x + n_2y + n_3z = 0$. Hence, the equation of the reflection plane is given by,

$$\boxed{n_1x + n_2y + n_3z = 0\,.} \tag{76}$$

Note that this equation for the reflection plane does not depend on the overall sign of $\hat{\boldsymbol{n}}$. This makes sense, as both $\hat{\boldsymbol{n}}$ and $-\hat{\boldsymbol{n}}$ are perpendicular to the reflection plane.

The equation for the reflection plane can also be derived directly as follows. In the case of $\theta = \pi$, the unit normal to the reflection plane $\hat{\boldsymbol{n}}$ is undefined so we exclude this case from further consideration. If $\theta \neq \pi$, then the reflection plane corresponding to the improper rotation $\overline{R}(\hat{\boldsymbol{n}},\theta)$ does not depend on θ. Thus, we can take $\theta = 0$ and consider $\overline{R}(\hat{\boldsymbol{n}})$ which represents a mirror reflection through the reflection plane. Any vector $\vec{\boldsymbol{v}} = (x,y,z)$ that lies in the reflection plane is unaffected by the reflection and thus satisfies

$$\overline{R}(\hat{\boldsymbol{n}})\vec{\boldsymbol{v}} = \vec{\boldsymbol{v}}\,. \tag{77}$$

Hence, eq. (77) provides an equation for the reflection plane, which in light of eq. (74) is explicitly given by,

$$\begin{pmatrix} 1-2n_1^2 & -2n_1n_2 & -2n_1n_3 \\ -2n_1n_2 & 1-2n_2^2 & -2n_2n_3 \\ -2n_1n_3 & -2n_2n_3 & 1-2n_3^2 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}\,. \tag{78}$$

The matrix equation, eq. (78), is equivalent to:

$$\begin{pmatrix} n_1^2 & n_1n_2 & n_1n_3 \\ n_1n_2 & n_2^2 & n_2n_3 \\ n_1n_3 & n_2n_3 & n_3^2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0\,. \tag{79}$$

Assume that $n_1 \neq 0$.[11] Applying two elementary row operations, the matrix equation given in eq. (79) can be transformed into reduced row echelon form,

$$\begin{pmatrix} n_1^2 & n_1n_2 & n_1n_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0\,.$$

The solutions to this equation are all x, y and z that satisfy $n_1x+n_2y+n_3z=0$, which reproduces the equation of the reflection plane quoted in eq. (76), as expected.

Appendix: Derivation of the Rodriguez formula

In this Appendix, we shall derive a formula for $R(\hat{\boldsymbol{n}},\theta)$. Consider the three dimensional rotation of a vector $\vec{\boldsymbol{x}}$ into a vector $\vec{\boldsymbol{x}}\,'$, which is described algebraically by the equation,

$$\vec{\boldsymbol{x}}\,' = R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{x}}\,, \quad \text{where } \|\vec{\boldsymbol{x}}'\| = \|\vec{\boldsymbol{x}}\|. \tag{80}$$

Since we are rotating the vector $\vec{\boldsymbol{x}}$ around an axis that is parallel to the unit vector $\hat{\boldsymbol{n}}$, it is convenient to decompose $\vec{\boldsymbol{x}}$ into a component parallel to $\hat{\boldsymbol{n}}$ and a component perpendicular to $\hat{\boldsymbol{n}}$. Such a decomposition has the following form,

$$\vec{\boldsymbol{x}} = \vec{\boldsymbol{x}}_\parallel + \vec{\boldsymbol{x}}_\perp\,, \quad \text{where } \vec{\boldsymbol{x}}_\parallel \equiv x_\parallel \hat{\boldsymbol{n}}. \tag{81}$$

Note that $\vec{\boldsymbol{x}}_\perp$ is vector that lives in the two-dimensional plane perpendicular to $\hat{\boldsymbol{n}}$, whereas $\vec{\boldsymbol{x}}_\parallel$ lives on a one-dimensional line parallel to $\hat{\boldsymbol{n}}$. In the above notation, the unbolded symbol $x_\parallel$ is the length of the vector $\vec{\boldsymbol{x}}_\parallel$.

One can obtain convenient formulae for $\vec{\boldsymbol{x}}_\parallel$ and $\vec{\boldsymbol{x}}_\perp$ in terms of $\vec{\boldsymbol{x}}$ and $\hat{\boldsymbol{n}}$ as follows. First, note that

$$\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}_\perp = 0\,, \qquad \hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}_\parallel = 0\,, \tag{82}$$

which are equivalent to the statements that $\vec{\boldsymbol{x}}_\perp$ is perpendicular to $\hat{\boldsymbol{n}}$ and $\vec{\boldsymbol{x}}_\parallel$ is parallel to $\hat{\boldsymbol{n}}$. If we now compute the dot product $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}$ using eqs. (81) and (82), then it follows that

$$\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}} = \hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}_\parallel = x_\parallel\,. \tag{83}$$

Substituting for $x_\parallel$ back in eq. (81) yields,

$$\vec{\boldsymbol{x}}_\parallel = \hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}})\,. \tag{84}$$

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[11] The case of $n_1 = 0$ can be treated separately. One can check that special cases such as this one do not modify the end result.

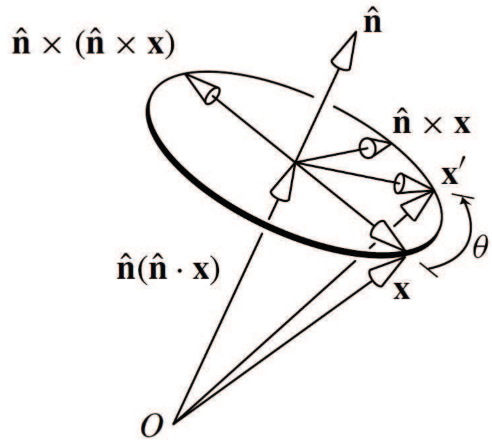

Figure 1: In the diagram above, the two-dimensional plane in which $\vec{\boldsymbol{x}}_\perp$ resides is indicated by the circular disk. We can designate this plane as the x–y plane, where the x-direction is parallel to $-\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})$ and the y-direction is parallel to $\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}}$. In light of eq. (87), the vector $\vec{\boldsymbol{x}}_\perp = -\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})$ points in the positive x-direction, and the vector $\vec{\boldsymbol{x}}'_\perp$ is obtained by a counterclockwise rotation of $\vec{\boldsymbol{x}}_\perp$ by an angle θ as exhibited above. This figure is taken from a lecture entitled *Representing Rotation* given by Matt Mason.

From this result, we can derive an equation for $\vec{\boldsymbol{x}}_\perp$. Using eqs. (81) and (84),

$$\vec{\boldsymbol{x}}_\perp = \vec{\boldsymbol{x}} - \vec{\boldsymbol{x}}_\parallel = \vec{\boldsymbol{x}} - \hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}})\,. \tag{85}$$

We can rewrite the above equation in a fancier way by using a well know vector identity [see eq. (3.8) of Chapter 6 on p. 280 of Boas], which yields

$$\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}) = \hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}) - \vec{\boldsymbol{x}}\,. \tag{86}$$

Hence, an equivalent form of eq. (85) is

$$\vec{\boldsymbol{x}}_\perp = -\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\,. \tag{87}$$

To derive a formula for $\vec{\boldsymbol{x}}\,' = R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{x}}$, the key observation is the following. By decomposing $\vec{\boldsymbol{x}}$ according to eq. (81), a rotation about an axis that points in the $\hat{\boldsymbol{n}}$ direction only rotates $\vec{\boldsymbol{x}}_\perp$, while leaving $\vec{\boldsymbol{x}}_\parallel$ unchanged. Since $\vec{\boldsymbol{x}}_\perp$ lives in a plane, all we need to do is to perform a two-dimensional rotation of $\vec{\boldsymbol{x}}_\perp$. The end result is the rotated vector,

$$\vec{\boldsymbol{x}}\,' = \vec{\boldsymbol{x}}'_\parallel + \vec{\boldsymbol{x}}'_\perp\,, \tag{88}$$

where $\vec{\boldsymbol{x}}'_\parallel = R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{x}}_\parallel = \vec{\boldsymbol{x}}_\parallel$ and $\vec{\boldsymbol{x}}'_\perp = R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{x}}_\perp$. This result is depicted in Figure 1.

Referring to Figures 1 and 2, we see that the rotated vector $\vec{\boldsymbol{x}}'_\perp$ is obtained by a counterclockwise rotation of $\vec{\boldsymbol{x}}_\perp$ by an angle θ in the two dimensional x–y plane. In order to check that Figure 2 makes sense as drawn, one should verify that $\vec{\boldsymbol{x}}_\perp$ is perpendicular to $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}$, and both these vectors are are mutually perpendicular to the unit vector $\hat{\boldsymbol{n}}$. Moreover, $\|\vec{\boldsymbol{x}}_\perp\| = \|\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}\|$ as indicated in Figure 2.

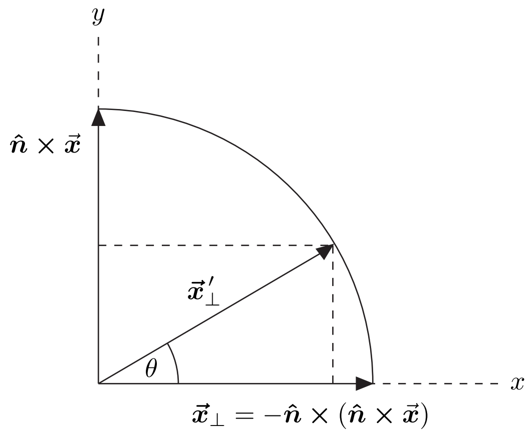

Figure 2: The rotated vector $\vec{\boldsymbol{x}}_\perp'$ is obtained by a counterclockwise rotation of $\vec{\boldsymbol{x}}_\perp$ by an angle θ in the two dimensional x–y plane. Note that $\|\vec{\boldsymbol{x}}_\perp'\| = \|\vec{\boldsymbol{x}}_\perp\| = \|\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}\|$. By projecting the vector $\vec{\boldsymbol{x}}_\perp'$ down to the x and y axes, it follows that $\vec{\boldsymbol{x}}_\perp' = (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\sin\theta - \big[\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\big]\cos\theta$.

It is convenient to define the following two unit vectors that point along the x and y axes, respectively,

$$\widehat{\boldsymbol{e}}_1 \equiv \frac{\vec{\boldsymbol{x}}_\perp}{\|\vec{\boldsymbol{x}}_\perp\|} = \frac{-\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})}{\|\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\|}\,, \qquad \widehat{\boldsymbol{e}}_2 \equiv \frac{\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}}{\|\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}\|}\,. \tag{89}$$

Note that $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\widehat{\boldsymbol{e}}_1 = \hat{\boldsymbol{n}}\boldsymbol{\cdot}\widehat{\boldsymbol{e}}_2 = 0$, since for any vector $\vec{\boldsymbol{A}}$ the cross product $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{A}}$ is perpendicular to $\hat{\boldsymbol{n}}$ by the definition of the cross product. Thus, $\widehat{\boldsymbol{e}}_1$ and $\widehat{\boldsymbol{e}}_2$ lie in the plane perpendicular to $\hat{\boldsymbol{n}}$ as required. To show that $\widehat{\boldsymbol{e}}_1$ and $\widehat{\boldsymbol{e}}_2$ are orthogonal, i.e., $\widehat{\boldsymbol{e}}_1\boldsymbol{\cdot}\widehat{\boldsymbol{e}}_2 = 0$, one can make use of eq. (86),

$$\big[\hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}) - \vec{\boldsymbol{x}}\big]\boldsymbol{\cdot}(\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}) = (\hat{\boldsymbol{n}} \cdot \vec{\boldsymbol{x}})\,\hat{\boldsymbol{n}}\boldsymbol{\cdot}(\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}) - \vec{\boldsymbol{x}}\boldsymbol{\cdot}(\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}) = 0\,, \tag{90}$$

where again we have noted that $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}$ is perpendicular both to $\hat{\boldsymbol{n}}$ and to $\vec{\boldsymbol{x}}$. Finally, in order to verify that $\|\vec{\boldsymbol{x}}_\perp\| = \|\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}\|$, we shall employ the well known vector identity, $\|\vec{\boldsymbol{A}} \times \vec{\boldsymbol{B}}\|^2 = \|\vec{\boldsymbol{A}}\|^2\|\vec{\boldsymbol{B}}\|^2 - (\vec{\boldsymbol{A}}\boldsymbol{\cdot}\vec{\boldsymbol{B}})^2$. It then follows that

$$\|\vec{\boldsymbol{x}}_\perp\|^2 = \|\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\|^2 = \|\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}\|^2 = \|\vec{\boldsymbol{x}}\|^2 - (\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}})^2\,, \tag{91}$$

after using the fact that the length of the unit vector $\|\hat{\boldsymbol{n}}\| = 1$ and $\hat{\boldsymbol{n}}\boldsymbol{\cdot}(\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}) = 0$.

Figure 2 provides a geometric method for finding an expression for $\vec{\boldsymbol{x}}_\perp'$ in terms of $\vec{\boldsymbol{x}}_\perp$. By projecting the vector $\vec{\boldsymbol{x}}_\perp'$ down to the x and y axes in Figure 2, it follows that $\vec{\boldsymbol{x}}_\perp'$ is the vector sum of the two projected vectors. That is,

$$\boxed{\vec{\boldsymbol{x}}_\perp' = (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\sin\theta - \big[\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})\big]\cos\theta\,.} \tag{92}$$

It is straightforward to verify that $\|\vec{\boldsymbol{x}}_\perp'\| = \|\vec{\boldsymbol{x}}_\perp\|$, which implies that a counterclockwise rotation of $\vec{\boldsymbol{x}}_\perp$ by an angle θ yields $\vec{\boldsymbol{x}}_\perp'$, as required. In particular, in light of eqs. (91) and (92), one can compute $\|\vec{\boldsymbol{x}}_\perp'\|^2 \equiv \vec{\boldsymbol{x}}_\perp'\boldsymbol{\cdot}\vec{\boldsymbol{x}}_\perp'$ as follows:[12]

$$\|\vec{\boldsymbol{x}}_\perp'\|^2 = \|\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}}\|^2\sin^2\theta + \|\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})\|^2\cos^2\theta = \|\vec{\boldsymbol{x}}_\perp\|^2(\sin^2\theta+\cos^2\theta) = \|\vec{\boldsymbol{x}}_\perp\|^2\,. \tag{93}$$

[12]In the computation shown in eq. (93), the cross term vanishes since $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}}$ and $\hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{x}})$ are perpendicular, which implies that their dot product is zero.

Finally, by using eq. (84),

$$\boxed{\vec{\boldsymbol{x}}_{\parallel}' = \vec{\boldsymbol{x}}_{\parallel} = \hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}})\,,} \tag{94}$$

since $\vec{\boldsymbol{x}}_{\parallel}$ lies along the direction of the axis of rotation, $\hat{\boldsymbol{n}}$, and thus does not rotate. Adding the results of eqs. (92) and (94), we conclude that

$$\vec{\boldsymbol{x}}\,' = \vec{\boldsymbol{x}}_{\parallel}' + \vec{\boldsymbol{x}}_{\perp}' = \hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}) + (\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})\sin\theta - \big[\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})\big]\cos\theta\,. \tag{95}$$

Eq. (95) is equivalent to to the equation $\vec{\boldsymbol{x}}\,' = R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{x}}$, where the matrix $R(\hat{\boldsymbol{n}},\theta)$ is given by eq. (52). To verify this assertion is a straightforward but tedious exercise in expanding out the components of the corresponding cross products. However, if you are comfortable in using the Levi-Civita epsilon symbol, then one can directly obtain the Rodriguez formula given in eq. (54) by writing out eq. (95) in terms of components. The components of the cross product are given by [see, e.g. eq. (5.11) of Chapter 10 on p. 511 of Boas],

$$(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})_i = -(\vec{\boldsymbol{x}}\times\hat{\boldsymbol{n}})_i = -\sum_{j=1}^{3}\sum_{k=1}^{3}\epsilon_{ijk}x_j n_k\,. \tag{96}$$

Similarly, using eq. (86),

$$\big[\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{x}})\big]_i = \big[\hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{x}}) - \vec{\boldsymbol{x}}\big]_i = n_i\left(\sum_{j=1}^{n} n_j x_j\right) - x_i\,. \tag{97}$$

Hence, the components of eq. (95) are,

$$\begin{aligned} x_i' &= n_i\left(\sum_{j=1}^{n} n_j x_j\right) - \sin\theta\sum_{j=1}^{3}\sum_{k=1}^{3}\epsilon_{ijk}x_j n_k - \cos\theta\left\{n_i\left(\sum_{j=1}^{n} n_j x_j\right) - x_i\right\} \\ &= x_i\cos\theta + \sum_{j=1}^{3}\left[(1-\cos\theta)n_i n_j - \sin\theta\sum_{k=1}^{3}\epsilon_{ijk}n_k\right]x_j \\ &= \sum_{j=1}^{3}\left[\delta_{ij} + (1-\cos\theta)n_i n_j - \sin\theta\sum_{k=1}^{3}\epsilon_{ijk}n_k\right]x_j\,, \end{aligned} \tag{98}$$

after employing the identity, $x_i = \sum_{j=1}^{3}\delta_{ij}x_j$. Comparing eq. (98) with eq. (80) written in component form,

$$x_i' = \sum_{j=1}^{3} R_{ij}(\hat{\boldsymbol{n}},\theta)x_j\,, \tag{99}$$

one can immediately read off the expression for $R_{ij}(\hat{\boldsymbol{n}},\theta)$,

$$R_{ij}(\hat{\boldsymbol{n}},\theta) = \delta_{ij} + (1-\cos\theta)n_i n_j - \sin\theta\sum_{k=1}^{3}\epsilon_{ijk}n_k\,, \tag{100}$$

which coincides with the Rodriguez formula given in eq. (54).