The Matrix Elements of a 3×3 Orthogonal Matrix—Revisited

1. Introduction

In a class handout entitled, *Three-Dimensional Proper and Improper Rotation Matrices*, I provided a derivation of the explicit form for most general 3×3 orthogonal matrix. A proper rotation matrix with determinant 1, denoted by $R(\hat{\boldsymbol{n}}, \theta)$, represents a counterclockwise rotation by an angle θ about a fixed axis $\hat{\boldsymbol{n}}$. An improper rotation with determinant -1, denoted by $\overline{R}(\hat{\boldsymbol{n}}, \theta)$ represents a reflection through a plane that passes through the origin and is perpendicular to a unit vector $\hat{\boldsymbol{n}}$ (called the normal to the reflection plane) together with a counterclockwise rotation by θ about $\hat{\boldsymbol{n}}$.

For example, the matrix representation of the counterclockwise rotation by an angle θ about a fixed z-axis is given by [cf. eq. (7.18) on p. 129 of Boas]:

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

Similarly, the matrix representation of a reflection through the x–y plane together with a counterclockwise rotation by an angle θ about a fixed z-axis (which points along the normal to the reflection plane) is given by [cf. eq. (7.19) on p. 129 of Boas]:

$$\overline{R}(\boldsymbol{k}, \theta) \equiv \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix} . \tag{2}$$

In these notes, I shall derive the general expressions for the matrix elements of $R(\hat{\boldsymbol{n}}, \theta)$ and $\overline{R}(\hat{\boldsymbol{n}}, \theta)$. These expressions have already been obtained in the class handout cited above. In contrast, I will provide here a much simpler derivation of the explicit forms for $R(\hat{\boldsymbol{n}}, \theta)$ and $\overline{R}(\hat{\boldsymbol{n}}, \theta)$, based on the techniques of tensor algebra.

2. A derivation of the Rodriguez formula

The matrix elements of $R(\hat{\boldsymbol{n}}, \theta)$ will be denoted by R_{ij}. Since $R(\hat{\boldsymbol{n}}, \theta)$ describes a rotation by an angle θ about an axis $\hat{\boldsymbol{n}}$, the formula for R_{ij} that we seek will depend on 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:

$$n_1^2 + n_2^2 + n_3^2 = 1\,. \tag{3}$$

Using the techniques of tensor algebra, we can derive the formula for R_{ij} in the following way. We can regard R_{ij} as the components of a second-rank tensor (see

Appendix A). Likewise, the n_i are components of a vector (equivalently, a first-rank tensor). Two other important quantities for the analysis are the *invariant* tensors δ_{ij} (the Kronecker delta) and ϵ_{ijk} (the Levi-Civita tensor). If we invoke the covariance of Cartesian tensor equations, then one must be able to express R_{ij} in terms of a second-rank tensor composed of n_i, δ_{ij} and ϵ_{ijk}, as there are no other tensors in the problem that could provide a source of indices. Thus, the form of the formula for R_{ij} must be:

$$R_{ij} = a\delta_{ij} + bn_in_j + c\epsilon_{ijk}n_k\,, \tag{4}$$

where there is an implicit sum over the index k in the third term of eq. (4).[1] The numbers a, b and c are real scalar quantities. As such, a, b and c are functions of θ, since the rotation angle is the only relevant scalar quantity in this problem.[2] If we also allow for transformations between right-handed and left-handed orthonormal coordinate systems, then R_{ij} and δ_{ij} are true second-rank tensors and ϵ_{ijk} is a third-rank pseudotensor. Thus, to ensure that eq. (4) is covariant with respect to transformations between two bases that are related by either a proper or an improper rotation, we conclude that a and b are true scalars, and the product $c\hat{\boldsymbol{n}}$ is a pseudovector.[3]

We now propose to deduce conditions that are satisfied by a, b and c. The first condition is obtained by noting that

$$R(\hat{\boldsymbol{n}},\theta)\hat{\boldsymbol{n}} = \hat{\boldsymbol{n}}\,. \tag{5}$$

This is clearly true, since $R(\hat{\boldsymbol{n}},\theta)$, when acting on a vector, rotates the vector around the axis $\hat{\boldsymbol{n}}$, whereas any vector parallel to the axis of rotation is invariant under the action of $R(\hat{\boldsymbol{n}},\theta)$. In terms of components

$$R_{ij}n_j = n_i\,. \tag{6}$$

To determine the consequence of this equation, we insert eq. (4) into eq. (6) and make use of eq. (3). Noting that[4]

$$\delta_{ij}n_j = n_i\,, \qquad n_jn_j = 1 \qquad \epsilon_{ijk}n_jn_k = 0\,, \tag{7}$$

[1] We follow the Einstein summation convention in these notes. That is, there is an implicit sum over any pair of repeated indices in the present and all subsequent formulae.

[2] One can also construct a scalar by taking the dot product of $\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}}$, but this quantity is equal to 1 [cf. eq. (3)], since $\hat{\boldsymbol{n}}$ is a unit vector.

[3] Under inversion of the coordinate system, $\theta \to -\theta$ and $\hat{\boldsymbol{n}} \to -\hat{\boldsymbol{n}}$. However, since $0 \leq \theta \leq \pi$ (by convention), we must then use eq. (12) to flip the signs of both θ and $\hat{\boldsymbol{n}}$ to represent the rotation $R(\hat{\boldsymbol{n}},\theta)$ in the new coordinate system. Hence, the signs of θ and $\hat{\boldsymbol{n}}$ effectively *do not change* under the inversion of the coordinate system. That is, θ is a true scalar and $\hat{\boldsymbol{n}}$ is a pseudovector, in which case c is also a true scalar. In a different convention where $-\pi \leq \theta \leq \pi$ (which we do not adopt in these notes), θ is a pseudoscalar and $\hat{\boldsymbol{n}}$ is a true vector, in which case c is also a pseudoscalar. Independent of these conventions, the product $c\hat{\boldsymbol{n}}$ is a pseudovector as asserted in the text above.

[4] In the third equation of eq. (7), there is an implicit sum over j and k. Since $\epsilon_{ijk} = -\epsilon_{jik}$, when the sum $\epsilon_{ijk}n_jn_k$ is carried out, we find that for every positive term, there is an identical negative term to cancel it. The total sum is therefore equal to zero. This is an example of a very general rule. Namely, one *always* finds that the product of two tensor quantities, one symmetric under the interchange of a pair of summed indices and one antisymmetric under the interchange of a pair of summed indices, is equal to zero when summed over the two indices. In the present case, n_jn_k is symmetric under the interchange of j and k, whereas ϵ_{ijk} is antisymmetric under the interchange of j and k. Hence their product, summed over j and k, is equal to zero.

it follows immediately that $n_i(a+b)=n_i$. Hence,

$$a+b=1\,. \tag{8}$$

Since the formula for R_{ij} given by eq. (4) must be completely general, it must hold for any special case. In particular, consider the case where $\hat{\boldsymbol{n}}=\boldsymbol{k}$. In this case, eqs. (1) and (4) yields:

$$R(\boldsymbol{k},\theta)_{11}=\cos\theta=a\,,\qquad\qquad R(\boldsymbol{k},\theta)_{12}=-\sin\theta=c\,\epsilon_{123}n_3=c\,. \tag{9}$$

Using eqs. (8) and (9) we conclude that,

$$a=\cos\theta\,,\qquad\quad b=1-\cos\theta\,,\qquad\quad c=-\sin\theta\,. \tag{10}$$

Inserting these results into eq. (4) yields the *Rodriguez formula*:

$$\boxed{R_{ij}(\hat{\boldsymbol{n}},\theta)=\cos\theta\,\delta_{ij}+(1-\cos\theta)n_in_j-\sin\theta\,\epsilon_{ijk}n_k} \tag{11}$$

We can write $R(\hat{\boldsymbol{n}},\theta)$ explicitly in 3×3 matrix form, although eq. (11) is more compact and convenient. Indeed, one can check that eq. (11) is equivalent to eq. (17) of the previous class handout, *Three-Dimensional Proper and Improper Rotation Matrices*.

The general rotation matrix $R(\hat{\boldsymbol{n}},\theta)$ given in eq. (11) satisfies the following two relations:

$$[R(\hat{\boldsymbol{n}},\theta)]^{-1}=R(\hat{\boldsymbol{n}},-\theta)=R(-\hat{\boldsymbol{n}},\theta)\,, \tag{12}$$

$$R(\hat{\boldsymbol{n}},2\pi-\theta)=R(-\hat{\boldsymbol{n}},\theta)\,, \tag{13}$$

which implies that any three-dimensional rotation can be described by a counterclockwise rotation by θ about an arbitrary axis $\hat{\boldsymbol{n}}$, where $0\leq\theta\leq\pi$. In this convention, the overall sign of $\hat{\boldsymbol{n}}$ is meaningful for $0<\theta<\pi$. In the case of $\theta=\pi$, we have

$$R_{ij}(\hat{\boldsymbol{n}},\pi)=R_{ij}(-\hat{\boldsymbol{n}},\pi)=2n_in_j-\delta_{ij}\,, \tag{14}$$

which means that $R(\hat{\boldsymbol{n}},\pi)$ and $R(-\hat{\boldsymbol{n}},\pi)$ represent the *same* rotation. Finally, if $\theta=0$ then $R_{ij}(\hat{\boldsymbol{n}},0)=\delta_{ij}$ is the identity operator, which is independent of the direction of $\hat{\boldsymbol{n}}$.

3. The matrix elements of an 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 is of the form:

$$\overline{R}(\hat{\boldsymbol{n}},\theta)\equiv R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}})=\overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}},\theta)\,, \tag{15}$$

where $\overline{R}(\hat{\boldsymbol{n}})$ is called a *reflection matrix*. In particular, $\overline{R}(\hat{\boldsymbol{n}})=\overline{R}(-\hat{\boldsymbol{n}})$ represents a mirror reflection through a plane passing through the origin that is normal to the unit vector $\hat{\boldsymbol{n}}$.[5] Note that the improper rotation defined in eq. (15) does not depend on the order in which the proper rotation and reflection are applied. It follows from eq. (15) that

$$\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(-\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}}, 0)\,, \tag{16}$$

after using $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$. Note that all reflection matrices are orthogonal matrices with $\det \overline{R}(\hat{\boldsymbol{n}}) = -1$, with the property that:

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

The matrix elements of $\overline{R}(\hat{\boldsymbol{n}}, \theta)$ will be denoted by $\overline{R}_{ij}$. The derivation of an explicit form for $\overline{R}(\hat{\boldsymbol{n}}, \theta)$ follows closely the derivation of $R(\hat{\boldsymbol{n}}, \theta)$ given in Section 1. In particular, we can also express $\overline{R}_{ij}$ in terms of a second-rank tensor composed of n_i, δ_{ij} and ϵ_{ijk}, since there are no other tensors in the problem that could provide a source of indices. Thus, the form of the formula for $\overline{R}_{ij}$ must be:

$$\overline{R}_{ij} = a\delta_{ij} + bn_i n_j + c\epsilon_{ijk} n_k\,, \tag{17}$$

where the coefficients of a, b and c need not be the same as those that appear in eq. (4).

In this case, a, b and c can be determined as follows. The first condition is obtained by noting that

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

This equation is true since any vector that is parallel to $\hat{\boldsymbol{n}}$ (which points along the normal to the reflection plane) is inverted (whereas the associated rotation about $\hat{\boldsymbol{n}}$ has no further effect). In terms of components

$$\overline{R}_{ij} n_j = -n_i\,. \tag{18}$$

To determine the consequence of this equation, we insert eq. (17) into eq. (18) and make use of eq. (3). using eq. (7), it follows immediately that $n_i(a + b) = -n_i$. Hence,

$$a + b = -1\,. \tag{19}$$

Since the formula for $\overline{R}_{ij}$ given by eq. (17) must be completely general, it must hold for any special case. In particular, consider the case where $\hat{\boldsymbol{n}} = \boldsymbol{k}$. In this case, eqs. (2) and (17) yields:

$$\overline{R}(\boldsymbol{k}, \theta)_{11} = \cos\theta = a\,, \qquad \overline{R}(\boldsymbol{k}, \theta)_{12} = -\sin\theta = c\,\epsilon_{123} n_3 = c\,. \tag{20}$$

Using eqs. (19) and (20) we conclude that,

$$a = \cos\theta\,, \qquad b = -1 - \cos\theta\,, \qquad c = -\sin\theta\,. \tag{21}$$

[5]Geometrically, it is clear that a mirror reflection is not sensitive to the sign of the normal to the reflection plane $\hat{\boldsymbol{n}}$.

Inserting these results into eq. (17) yields the analog of the Rodriguez formula for improper rotation matrices:

$$\boxed{\overline{R}_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} - (1+\cos\theta)n_i n_j - \sin\theta\,\epsilon_{ijk}n_k} \tag{22}$$

We can write $\overline{R}(\hat{\boldsymbol{n}},\theta)$ explicitly in 3×3 matrix form, although eq. (22) is more compact and convenient. Indeed, one can check that eq. (22) is equivalent to eq. (47) of the previous class handout, *Three-Dimensional Proper and Improper Rotation Matrices.*

The general improper rotation matrix $\overline{R}(\hat{\boldsymbol{n}},\theta)$ given in eq. (22) satisfies the following two relations:

$$[\overline{R}(\hat{\boldsymbol{n}},\theta)]^{-1} = \overline{R}(\hat{\boldsymbol{n}},-\theta) = \overline{R}(-\hat{\boldsymbol{n}},\theta)\,, \tag{23}$$

$$\overline{R}(\hat{\boldsymbol{n}},2\pi-\theta) = \overline{R}(-\hat{\boldsymbol{n}},\theta)\,, \tag{24}$$

which implies that any three-dimensional improper rotation can be described by a reflection through a plane that passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$, together with a counterclockwise rotation by θ about $\hat{\boldsymbol{n}}$, where $0\leq\theta\leq\pi$. In this convention, the overall sign of $\hat{\boldsymbol{n}}$ is meaningful for $0<\theta<\pi$. In the case of $\theta=0$, the improper rotation matrix

$$\overline{R}(\hat{\boldsymbol{n}},0) = \overline{R}(-\hat{\boldsymbol{n}},0) = \delta_{ij} - 2n_i n_j\,,$$

corresponds to the reflection matrix $R(\hat{\boldsymbol{n}})$ defined in eq. (16). Indeed, $\overline{R}(\hat{\boldsymbol{n}},0)$ and $\overline{R}(-\hat{\boldsymbol{n}},0)$ represent the *same* reflection. Finally, if $\theta=\pi$ then $\overline{R}_{ij}(\hat{\boldsymbol{n}},\pi)=-\delta_{ij}$ is the inversion operator, which is independent of the direction of $\hat{\boldsymbol{n}}$.

4. Determining the properties of a general 3 × 3 orthogonal matrix

The results obtained in eqs. (11) and (22) can be expressed as a single equation. Consider a general 3×3 orthogonal matrix R, corresponding to *either* a proper or improper rotation. Then its matrix elements are given by:

$$R_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} + (\varepsilon-\cos\theta)n_i n_j - \sin\theta\,\epsilon_{ijk}n_k\,, \tag{25}$$

where

$$\varepsilon \equiv \det R(\hat{\boldsymbol{n}},\theta)\,. \tag{26}$$

That is, $\varepsilon=1$ for a proper rotation and $\varepsilon=-1$ for an improper rotation. Using eq. (25), one can derive expressions for the unit vector $\hat{\boldsymbol{n}}$ and the angle θ in terms of the matrix elements of R. With some tensor algebra manipulations involving the Levi-Civita tensor, we can quickly obtain the desired results.

First, we compute the trace of $R(\hat{\boldsymbol{n}},\theta)$. In particular, using eq. (25) it follows that:[6]

$$\mathrm{Tr}\ R(\hat{\boldsymbol{n}},\theta) \equiv R_{ii} = \varepsilon + 2\cos\theta\,. \tag{27}$$

[6]Since we are employing the Einstein summation convention, the quantities $R_{ii}\equiv\mathrm{Tr}\ R$ and $\delta_{ii}\equiv\mathrm{Tr}\,\mathbf{I}$ each involve an implicit sum over i, and thus define the trace of R and $\mathbf{I}$, respectively.

In deriving this result, we used the fact that $\delta_{ii} = \mathrm{Tr}\,\mathbf{I} = 3$ (since the indices run over $i = 1, 2, 3$ in three-dimensional space) and $\epsilon_{iik} = 0$ (the latter is a consequence of the fact that the Levi-Civita tensor is totally antisymmetric under the interchange of any two indices). By convention, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. Thus,

$$\cos\theta = \tfrac{1}{2}\left(\mathrm{Tr}\,R - \varepsilon\right) \quad \text{and} \quad \sin\theta = (1-\cos^2\theta)^{1/2} = \tfrac{1}{2}\sqrt{(3-\varepsilon\,\mathrm{Tr}\,R)(1+\varepsilon\,\mathrm{Tr}\,R)}\,, \tag{28}$$

where $\cos\theta$ is determined from eq. (27) and we have used $\varepsilon^2 = 1$. All that remains is to determine the unit vector $\hat{\boldsymbol{n}}$.

Let us multiply eq. (11) by ϵ_{ijm} and sum over i and j. Noting that[7]

$$\epsilon_{ijm}\delta_{ij} = \epsilon_{ijm}n_i n_j = 0\,, \qquad \epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}\,, \tag{29}$$

it follows that

$$2n_m \sin\theta = -R_{ij}\epsilon_{ijm}\,. \tag{30}$$

If R is a symmetric matrix (i.e. $R_{ij} = R_{ji}$), then $R_{ij}\epsilon_{ijm} = 0$ automatically since ϵ_{ijk} is antisymmetric under the interchange of the indices i and j. In this case $\sin\theta = 0$ and we must seek other means to determine $\hat{\boldsymbol{n}}$. If $\sin\theta \neq 0$, then one can divide both sides of eq. (30) by $\sin\theta$. Using eq. (28), we obtain:

$$n_m = -\frac{R_{ij}\epsilon_{ijm}}{2\sin\theta} = \frac{-R_{ij}\epsilon_{ijm}}{\sqrt{(3-\varepsilon\,\mathrm{Tr}\,R)(1+\varepsilon\,\mathrm{Tr}\,R)}}\,, \qquad \sin\theta \neq 0\,. \tag{31}$$

More explicitly,

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{(3-\varepsilon\,\mathrm{Tr}\,R)(1+\varepsilon\,\mathrm{Tr}\,R)}}\Big(R_{32}-R_{23}\,,\; R_{13}-R_{31}\,,\; R_{21}-R_{12}\Big)\,, \qquad \varepsilon\,\mathrm{Tr}R \neq -1\,,\,3\,. \tag{32}$$

In Appendix B, we verify that $\hat{\boldsymbol{n}}$ as given by eq. (31) is a vector of unit length [as required by eq. (3)]. The overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (31) due to our convention in which $\sin\theta \geq 0$. If we multiply eq. (30) by n_m and sum over m, then

$$\sin\theta = -\tfrac{1}{2}\epsilon_{ijm}R_{ij}n_m\,, \tag{33}$$

after using $n_m n_m = 1$. This provides an additional check on the determination of the rotation angle.

Alternatively, we can define a matrix S whose matrix elements are given by:

$$\begin{aligned} S_{jk} &\equiv R_{jk} + R_{kj} + (\varepsilon - \mathrm{Tr}\,R)\delta_{jk} \qquad (34)\\ &= 2(\varepsilon - \cos\theta)n_j n_k = (3\varepsilon - \mathrm{Tr}\,R)n_j n_k\,, \end{aligned}$$

[7] As discussed in footnote 4, the identity $\epsilon_{ijm}n_i n_j = 0$ arises because ϵ_{ijm} is antisymmetric and $n_i n_j$ is symmetric under the interchange of i and j. Summing over the repeated indices i and j then yields an equal number of positive and negative terms that cancel exactly. To derive the second identity of eq. (29), one can set $j = \ell$ in eq. (38) and then sum over the repeated index ℓ. Relabeling the indices of the resulting sum then gives the identity $\epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}$.

after using eq. (25) for R_{jk}. Hence,[8]

$$n_j n_k = \frac{S_{jk}}{3\varepsilon - \operatorname{Tr} R}\,, \qquad \operatorname{Tr} R \neq 3\varepsilon\,. \tag{35}$$

To determine $\hat{\boldsymbol{n}}$ up to an overall sign, we simply set $j = k$ (no sum) in eq. (35), which fixes the value of n_j^2. If $\sin\theta \neq 0$, the overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (30).

As noted above, if R is a symmetric matrix (i.e. $R_{ij} = R_{ji}$), then $\sin\theta = 0$ and $\hat{\boldsymbol{n}}$ cannot be determined from eq. (31). In this case, eq. (27) determines whether $\cos\theta = +1$ or $\cos\theta = -1$. If $\cos\theta = \varepsilon$, then $R_{ij} = \varepsilon\delta_{ij}$, in which case $S = \mathbf{0}$ and the axis $\hat{\boldsymbol{n}}$ is undefined. For $\cos\theta = -\varepsilon$, one can determine $\hat{\boldsymbol{n}}$ up to an overall sign using eq. (35) as noted above. In this case, the ambiguity in the overall sign of $\hat{\boldsymbol{n}}$ is immaterial, in light of eq. (14).

To summarize, eqs. (28), (32) and (35) provide a simple algorithm for determining the unit vector $\hat{\boldsymbol{n}}$ and the rotation angle θ for any proper or improper rotation matrix $R(\hat{\boldsymbol{n}},\theta) \neq \varepsilon\mathbf{I}$.

Finally, one additional property of three-dimensional proper rotation matrices is especially noteworthy:

$$R(\hat{\boldsymbol{n}},\theta) = PR(\hat{\boldsymbol{n}}',\theta)P^{-1}\,, \qquad \text{for } \hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}', \text{ where } P \text{ is a proper rotation matrix.} \tag{36}$$

A proof that employs the methods of tensor algebra is given in Appendix C.

Appendix A: Matrix elements of matrices correspond to the components of second rank tensors

In the class handout entitled, *Vector coordinates, matrix elements and changes of basis*, we examined how the matrix elements of linear operators change under a change of basis. Consider the matrix elements of a linear operator with respect to two different orthonormal bases, $\mathcal{B} = \{\hat{\boldsymbol{e}}_1\,,\,\hat{\boldsymbol{e}}_2\,,\,\hat{\boldsymbol{e}}_3\}$ and $\mathcal{B}' = \{\hat{\boldsymbol{e}}'_1\,,\,\hat{\boldsymbol{e}}'_2\,,\,\hat{\boldsymbol{e}}'_3\}$. Then, using the Einstein summation convention,

$$\hat{\boldsymbol{e}}'_j = P_{ij}\hat{\boldsymbol{e}}_i\,,$$

where P is an orthogonal matrix. Given any linear operator A with matrix elements a_{ij} with respect to the basis $\mathcal{B}$, the matrix elements a'_{ij} with respect to the basis $\mathcal{B}'$ are given by

$$a'_{k\ell} = (P^{-1})_{ki}a_{ij}P_{j\ell} = P_{ik}a_{ij}P_{j\ell}\,,$$

where we have used the fact that $P^{-1} = P^{\mathsf{T}}$ in the second step above. Finally, identifying $P = R^{-1}$, where R is also an orthogonal matrix, it follows that

$$a'_{k\ell} = R_{ki}R_{\ell j}a_{ij}\,,$$

which we recognize as the transformation law for the components of a second rank Cartesian tensor.

[8] Eq. (34) yields $\operatorname{Tr} S = 3\varepsilon - \operatorname{Tr} R$. One can then use eq. (35) to verify that $\hat{\boldsymbol{n}}$ is a unit vector.

Appendix B: Verifying that $\hat{\boldsymbol{n}}$ obtained from eq. (31) is a unit vector

We first need some preliminary results. Using the results from the handout entitled, *The Characteristic Polynomial*, the characteristic equation of an arbitrary 3×3 matrix R is given by:

$$p(\lambda) = -\left[\lambda^3 - \lambda^2 \text{Tr } R + c_2\lambda - \det R\right] ,$$

where

$$c_2 = \tfrac{1}{2}\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] .$$

For an orthogonal matrix, $\varepsilon \equiv \det R = \pm 1$. Hence,

$$p(\lambda) = -\left[\lambda^3 - \lambda^2 \text{Tr } R + \tfrac{1}{2}\lambda\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] - \varepsilon\right] .$$

We now employ the Cayley-Hamilton theorem, which states that a matrix satisfies its own characteristic equation, i.e. $p(R) = 0$. Hence,

$$R^3 - R^2\,\text{Tr } R + \tfrac{1}{2}R\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] - \varepsilon\mathbf{I} = 0\,.$$

Multiplying the above equation by R^{-1}, and using the fact that $R^{-1} = R^{\mathsf{T}}$ for an orthogonal matrix,

$$R^2 - R\,\text{Tr } R + \tfrac{1}{2}\mathbf{I}\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] - \varepsilon R^{\mathsf{T}} = 0\,.$$

Finally, we take the trace of the above equation. Using $\text{Tr}(R^{\mathsf{T}}) = \text{Tr } R$, we can solve for $\text{Tr}(R^2)$. Using $\text{Tr } \mathbf{I} = 3$, the end result is given by:

$$\text{Tr}(R^2) = (\text{Tr } R)^2 - 2\varepsilon\,\text{Tr}\,R\,, \tag{37}$$

which is satisfied by all 3×3 orthogonal matrices.

We now verify that $\hat{\boldsymbol{n}}$ as determined from eq. (31) is a unit vector. For convenience, we repeat eq. (31) here:

$$n_m = -\tfrac{1}{2}\frac{R_{ij}\epsilon_{ijm}}{\sin\theta} = \frac{-R_{ij}\epsilon_{ijm}}{\sqrt{(3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})}}\,, \qquad \sin\theta \neq 0\,,$$

where $R_{ii} \equiv \text{Tr } R$. We evaluate $\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}} = n_m n_m$ as follows:

$$n_m n_m = \frac{R_{ij}\epsilon_{ijm}R_{k\ell}\epsilon_{k\ell m}}{(3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})} = \frac{R_{ij}R_{k\ell}(\delta_{ik}\delta_{j\ell} - \delta_{i\ell}\delta_{jk})}{(3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})} = \frac{R_{ij}R_{ij} - R_{ij}R_{ji}}{(3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})}\,,$$

after making use of the identity given in eq. (5.8) on p. 510 of Boas,

$$\epsilon_{ijm}\epsilon_{k\ell m} = \delta_{ik}\delta_{j\ell} - \delta_{i\ell}\delta_{jk}\,. \tag{38}$$

The numerator of the above expression is equal to:

$$\begin{aligned} R_{ij}R_{ij} - R_{ij}R_{ji} &= \text{Tr}(R^{\mathsf{T}}R) - \text{Tr}(R^2) = \text{Tr } \mathbf{I} - \text{Tr}(R^2) \\ &= 3 - \text{Tr}(R^2) = 3 - (\text{Tr}\,R)^2 + 2\varepsilon\,\text{Tr}\,R \\ &= (3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})\,, \end{aligned} \tag{39}$$

after using eq. (37) for $\text{Tr}(R^2)$. Hence, employing eq. (39) in the expression for $n_m n_m$ above yields

$$\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}} = n_m n_m = \frac{R_{ij}R_{ij} - R_{ij}R_{ji}}{(3-\varepsilon\,R_{ii})(1+\varepsilon\,R_{ii})} = 1\,,$$

and the proof is complete.

Appendix C: Proof of the theorem given in eq. (36)

In this appendix, we prove the following theorem for proper three-dimensional rotation matrices,

$$R(\hat{\boldsymbol{n}},\theta) = PR(\hat{\boldsymbol{n}}',\theta)P^{-1}\,, \qquad \text{for } \hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}',\text{ where } P \text{ is a proper rotation matrix.} \tag{40}$$

To prove eq. (40), we first compute the angle of the rotation $PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$ using eq. (28) with $\varepsilon = 1$. Since $\mathrm{Tr}[PR(\hat{\boldsymbol{n}}',\theta)P^{-1}] = \mathrm{Tr}\,R(\hat{\boldsymbol{n}}',\theta)$ using the cyclicity of the trace, it follows that the angles of rotation corresponding to $PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$ and $R(\hat{\boldsymbol{n}}',\theta)$ coincide and are both equal to θ. To compute the corresponding axis of rotation $\hat{\boldsymbol{n}}$, we employ eq. (30),

$$2n_m \sin\theta = -(PR'P^{-1})_{ij}\epsilon_{ijm}\,, \tag{41}$$

where $R' \equiv R(\hat{\boldsymbol{n}}',\theta)$. Since P is a rotation matrix, we have $P^{-1} = P^{\mathsf{T}}$, or equivalently $(P^{-1})_{\ell j} = P_{j\ell}$. Hence, we can rewrite eq. (41) as:

$$2n_m \sin\theta = -P_{ik}R'_{k\ell}P_{j\ell}\epsilon_{ijm}\,. \tag{42}$$

Multiplying both sides of eq. (42) by P_{mn} and using the definition of the determinant of a 3×3 matrix,

$$P_{ik}P_{j\ell}P_{mn}\epsilon_{ijm} = (\det P)\epsilon_{k\ell n}\,,$$

it then follows that:

$$2P_{mn}n_m \sin\theta = -R'_{k\ell}\epsilon_{k\ell n}\,. \tag{43}$$

after noting that $\det P = 1$ (since P is a *proper* rotation matrix). Finally, we again use eq. (30) which yields

$$2n'_n \sin\theta = -R'_{k\ell}\epsilon_{k\ell n}\,. \tag{44}$$

Assuming that $\sin\theta \neq 0$, we can subtract eqs. (43) and (44) and divide out by $2\sin\theta$. Using $(P^{\mathsf{T}})_{nm} = P_{mn}$, the end result is:

$$\hat{\boldsymbol{n}}' - P^{\mathsf{T}}\hat{\boldsymbol{n}} = 0\,.$$

Since $PP^{\mathsf{T}} = P^{\mathsf{T}}P = \mathbf{I}$, we conclude that

$$\hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}'\,. \tag{45}$$

The case of $\sin\theta = 0$ must be treated separately. Using eq. (5), one can determine the axis of rotation $\hat{\boldsymbol{n}}$ of the rotation matrix $PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$ up to an overall sign. Since $R(\hat{\boldsymbol{n}}',\theta)\hat{\boldsymbol{n}}' = \hat{\boldsymbol{n}}'$, the following eigenvalue equation is obtained:

$$PR(\hat{\boldsymbol{n}}',\theta)P^{-1}(P\hat{\boldsymbol{n}}') = PR(\hat{\boldsymbol{n}}',\theta)\hat{\boldsymbol{n}}' = P\hat{\boldsymbol{n}}'\,. \tag{46}$$

That is, $P\hat{\boldsymbol{n}}'$ is an eigenvector of $PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$ with eigenvalue $+1$. It then follows that $P\hat{\boldsymbol{n}}'$ is the normalized eigenvector of $PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$ up to an overall undetermined sign. For $\sin\theta \neq 0$, the overall sign is fixed and is positive by eq. (45). If $\sin\theta = 0$, then there are two cases to consider. If $\theta = 0$, then $R(\hat{\boldsymbol{n}},0) = R(\hat{\boldsymbol{n}}',0) = \mathbf{I}$ and eq. (40) is trivially satisfied. If $\theta = \pi$, then eq. (14) implies that the unit vector parallel to the rotation axis is only defined up to an overall sign. Hence, eq. (45) is valid even in the case of $\sin\theta = 0$, and the proof is complete.