Eigenvalues and eigenvectors of rotation matrices

These notes are a supplement to a previous class handout entitled, *Rotation Matrices in two, three and many dimensions*. In these notes, we shall focus on the eigenvalues and eigenvectors of proper and improper rotation matrices in two and three dimensions.

1. The eigenvalues and eigenvectors of proper and improper rotation matrices in two dimensions

In the previous class handout cited above, we showed that the most general proper rotation matrix in two-dimensions is of the form,

$$R(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\,, \quad \text{where } 0 \leq \theta < 2\pi\,, \tag{1}$$

which represents a proper counterclockwise rotation by an angle θ in the x–y plane. Consider the eigenvalue problem,

$$R(\theta)\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}\,. \tag{2}$$

Since $R(\theta)$ rotates the vector $\vec{\boldsymbol{v}}$ by an angle θ, we conclude that for $\theta \neq 0 \pmod{\pi}$, there are no real eigenvectors $\vec{\boldsymbol{v}}$ that are solutions to eq. (2). This can be easily checked by an explicit calculation as follows.

$$\det(R(\theta) - \lambda\mathbf{I}) = 0 \quad \Longrightarrow \quad \det\begin{pmatrix} \cos\theta - \lambda & -\sin\theta \\ \sin\theta & \cos\theta - \lambda \end{pmatrix} = 0\,, \tag{3}$$

which yields the characteristic equation,

$$(\cos\theta - \lambda)^2 + \sin^2\theta = 0\,. \tag{4}$$

This equation simplifies to

$$\lambda^2 - 2\lambda\cos\theta + 1 = 0\,, \tag{5}$$

which yields the eigenvalues,

$$\lambda = \cos\theta \pm \sqrt{\cos^2\theta - 1} = \cos\theta \pm i\sin\theta = e^{\pm i\theta}\,. \tag{6}$$

Thus, we ave confirmed that the eigenvalues are not real if $\theta \neq 0 \pmod{\pi}$. For the special cases of $R = \mathbf{I}$ and $R = -\mathbf{I}$, corresponding to $\theta = 0$ and π, respectively, we obtain real eigenvalues as expected. In particular, the case of $\theta = \pi$ corresponds to a two dimension inversion $\vec{\boldsymbol{x}} \to -\vec{\boldsymbol{x}}$, which implies that the eigenvalue of $R(\pi)$ is doubly degenerate and equal to -1.

The case of improper rotations in two dimensions is more interesting. In the previous class handout cited above, we noted that the most general improper rotation matrix in two-dimensions is of the form,

$$\overline{R}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \quad \text{where } 0 \leq \theta < 2\pi\,, \tag{7}$$

which can be expressed as the product of a proper rotation and a reflection,

$$\overline{R} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{8}$$

However, it is easy to show that the action of $\overline{R}(\theta)$ is equivalent to a pure reflection through a line that passes through the origin. This can be seen by considering the eigenvalue problem,

$$\overline{R}(\theta)\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}\,. \tag{9}$$

We can again determine the eigenvalues of $\overline{R}(\theta)$ by solving its characteristic equation,

$$\det(\overline{R}(\theta) - \lambda\mathbf{I}) = 0 \quad \Longrightarrow \quad \det\begin{pmatrix} \cos\theta - \lambda & \sin\theta \\ \sin\theta & -\cos\theta - \lambda \end{pmatrix} = 0\,, \tag{10}$$

which is equivalent to

$$(\cos\theta - \lambda)(-\cos\theta - \lambda) - \sin^2\theta = 0\,. \tag{11}$$

This equation simplifies to

$$\lambda^2 - 1 = 0\,, \tag{12}$$

which yields the eigenvalues, $\lambda = \pm 1$.

The interpretation of this result is immediate. The matrix $\overline{R}(\theta)$ when operating on a vector $\vec{\boldsymbol{v}}$ represents a reflection of that vector through a line of reflection that passes through the origin. In the case of $\lambda = 1$ we have $\overline{R}(\theta)\vec{\boldsymbol{v}} = \vec{\boldsymbol{v}}$, which means that $\vec{\boldsymbol{v}}$ is a vector that lies parallel to the line of reflection (and is thus unaffected by the reflection). In the case of $\lambda = -1$ we have $\overline{R}(\theta)\vec{\boldsymbol{v}} = -\vec{\boldsymbol{v}}$, which means that $\vec{\boldsymbol{v}}$ is a vector that is perpendicular to the line of reflection (and is thus is transformed, $\vec{\boldsymbol{v}} \to -\vec{\boldsymbol{v}}$, by the reflection).

One can therefore determine the line of reflection by computing the eigenvector that corresponds to $\lambda = 1$,

$$\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix}. \tag{13}$$

If $\theta = 0 \pmod{2\pi}$, then any vector of the form $\left(\begin{smallmatrix} x \\ 0 \end{smallmatrix}\right)$ is an eigenvector corresponding to the eigenvalue $\lambda = 1$. This implies that the line of reflection is the x-axis, which corresponds to the equation $y = 0$. In general (for any value of θ), the solution to eq. (13) is

$$x\cos\theta + y\sin\theta = x\,, \tag{14}$$

or equivalently,

$$x(1-\cos\theta)-y\sin\theta=0\,. \tag{15}$$

It is convenient to use trigonometric identities to rewrite eq. (15) as

$$2x\sin^2\bigl(\tfrac{1}{2}\theta\bigr)-2y\sin\bigl(\tfrac{1}{2}\theta\bigr)\cos\bigl(\tfrac{1}{2}\theta\bigr)=0\,. \tag{16}$$

If $\theta\neq 0 \pmod{2\pi}$, then we can divide both sides of eq. (16) by $\sin\bigl(\tfrac{1}{2}\theta\bigr)$ to obtain[1]

$$x\sin\bigl(\tfrac{1}{2}\theta\bigr)-y\cos\bigl(\tfrac{1}{2}\theta\bigr)=0\,. \tag{17}$$

We recognize eq. (17) as an equation for a straight line that passes through the origin with a slope equal to $\tan\bigl(\tfrac{1}{2}\theta\bigr)$. Thus, we have demonstrated that the most general 2×2 orthogonal matrix with determinant equal to -1 given by $\overline{R}(\theta)$ represents a pure reflection through a straight line of slope $\tan\bigl(\tfrac{1}{2}\theta\bigr)$ that passes through the origin.

Finally, it is worth noting that since $\overline{R}(\theta)$ is both an orthogonal matrix, $\overline{R}(\theta)\overline{R}(\theta)^{\mathsf{T}}=\mathbf{I}$, and a symmetric matrix, $\overline{R}(\theta)^{\mathsf{T}}=\overline{R}(\theta)$, it follows that

$$\bigl[\overline{R}(\theta)\bigr]^2=\mathbf{I}\,, \tag{18}$$

which is property that must be satisfied by a reflection matrix since two consecutive reflections are equivalent to the identity operation when acting on a vector.

3. The eigenvalues and eigenvectors of proper rotation matrices in three dimensions

The most general three-dimensional proper rotation matrix, 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 $\hat{\boldsymbol{n}}$. All possible proper rotations correspond to $0\leq\theta\leq\pi$ and the unit vector $\hat{\boldsymbol{n}}$ pointing in any direction.

To learn more about the properties of a general three-dimensional rotation, consider the matrix representation $R(\hat{\boldsymbol{n}},\theta)$ with respect to the standard basis $\mathcal{B}_s=\{\boldsymbol{i}\,,\,\boldsymbol{j}\,,\,\boldsymbol{k}\}$. We can define a new coordinate system in which the unit vector $\hat{\boldsymbol{n}}$ points in the direction of the new z-axis; the corresponding new basis will be denoted by $\mathcal{B}'$. The matrix representation of the rotation with respect to $\mathcal{B}'$ is then given by

$$R(\boldsymbol{k},\theta)\equiv\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix}\,, \tag{19}$$

where the axis of rotation points in the z-direction (i.e., along the unit vector $\boldsymbol{k}$).

[1]Note that for $\theta=0 \pmod{2\pi}$, eq. (17) reduces to $y=0$ which is the equation for the x-axis, as expected.

Using the formalism developed in the class handout, *Vector coordinates, matrix elements, changes of basis, and matrix diagonalization*, there exists an invertible matrix P such that

$$R(\hat{\boldsymbol{n}},\theta) = PR(\boldsymbol{k},\theta)P^{-1}\,, \tag{20}$$

where $R(\boldsymbol{k},\theta)$ is given by eq. (19). In Appendix A, we will determine an explicit form for the matrix P. However, the mere existence of the matrix P in eq. (20) is sufficient to provide a simple algorithm for determining the rotation axis $\hat{\boldsymbol{n}}$ (up to an overall sign) and the rotation angle θ that characterize a general three-dimensional rotation matrix.

To determine the rotation angle θ, we note that the properties of the trace imply that $\mathrm{Tr}(PRP^{-1}) = \mathrm{Tr}(P^{-1}PR) = \mathrm{Tr}\,R$, since one can cyclically permute the matrices within the trace without modifying its value. Hence, it immediately follows from eq. (20) that

$$\mathrm{Tr}\ R(\hat{\boldsymbol{n}},\theta) = \mathrm{Tr}\ R(\boldsymbol{k},\theta) = 2\cos\theta + 1\,, \tag{21}$$

after taking the trace of eq. (19). By convention, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. Hence, the rotation angle is uniquely determined by eq. (21) To identify $\hat{\boldsymbol{n}}$, we observe that any vector that is parallel to the axis of rotation is unaffected by the rotation itself. This last statement can be expressed as an eigenvalue equation,

$$R(\hat{\boldsymbol{n}},\theta)\hat{\boldsymbol{n}} = \hat{\boldsymbol{n}}\,. \tag{22}$$

Thus, $\hat{\boldsymbol{n}}$ is an eigenvector of $R(\hat{\boldsymbol{n}},\theta)$ corresponding to the eigenvalue 1. In particular, the eigenvalue 1 is nondegenerate for any $\theta \neq 0$, in which case $\hat{\boldsymbol{n}}$ can be determined up to an overall sign by computing the eigenvalues and the normalized eigenvectors of $R(\hat{\boldsymbol{n}},\theta)$. A simple proof of this result is given in Appendix B. Here, we shall establish this assertion by noting that the eigenvalues of any matrix are invariant with respect to a similarity transformation. In light of eq. (20), it follows that the eigenvalues of $R(\hat{\boldsymbol{n}},\theta)$ are identical to the eigenvalues of $R(\boldsymbol{k},\theta)$. The latter can be obtained from the characteristic equation,

$$(1-\lambda)\left[(\cos\theta-\lambda)^2 + \sin^2\theta\right] = 0\,,$$

which simplifies to:

$$(1-\lambda)(\lambda^2 - 2\lambda\cos\theta + 1) = 0\,,$$

after using $\sin^2\theta + \cos^2\theta = 1$. Using the results of eqs. (5) and (6), it follows that the three eigenvalues of $R(\boldsymbol{k},\theta)$ are given by,

$$\lambda_1 = 1\,,\quad \lambda_2 = e^{i\theta}\,,\quad \lambda_3 = e^{-i\theta}\,,\qquad \text{for}\ \ 0 \leq \theta \leq \pi\,.$$

There are three distinct cases:

Case 1:	$\theta = 0$	$\lambda_1 = \lambda_2 = \lambda_3 = 1\,,$	$R(\hat{\boldsymbol{n}},0) = \mathbf{I}\,,$
Case 2:	$\theta = \pi$	$\lambda_1 = 1\,,\ \lambda_2 = \lambda_3 = -1\,,$	$R(\hat{\boldsymbol{n}},\pi)\,,$
Case 3:	$0 < \theta < \pi$	$\lambda_1 = 1, \lambda_2 = e^{i\theta}\,,\ \lambda_3 = e^{-i\theta}\,,$	$R(\hat{\boldsymbol{n}},\theta)\,,$

where the corresponding rotation matrix is indicated for each of the three cases.

For $\theta \neq 0$ the eigenvalue 1 is nondegenerate, as expected from the geometric interpretation that led to eq. (22). Moreover, the other two eigenvalues are complex conjugates of each other, whose real part is equal to $\cos\theta$, which uniquely fixes the rotation angle in the convention where $0 \leq \theta \leq \pi$. Case 1 corresponds to the identity (i.e. no rotation) and Case 2 corresponds to a 180° rotation about the axis $\hat{\boldsymbol{n}}$. In Case 2, the interpretation of the the doubly degenerate eigenvalue -1 is clear. Namely, the corresponding two linearly independent eigenvectors span the plane that passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. In particular, the two eigenvectors corresponding to the doubly degenerate eigenvalues, as well as any linear combination of these eigenvectors (which we shall denote generically by $\vec{\boldsymbol{v}}$) that lies in the plane perpendicular to $\hat{\boldsymbol{n}}$, are inverted by the 180° rotation and hence must satisfy $R(\hat{\boldsymbol{n}},\pi)\vec{\boldsymbol{v}} = -\vec{\boldsymbol{v}}$.

Since $\hat{\boldsymbol{n}}$ is a real vector of unit length, it is determined only up to an overall sign by eq. (22) when its corresponding eigenvalue 1 is nondegenerate. This sign ambiguity is immaterial in Case 2 given that $R(\hat{\boldsymbol{n}},\pi) = R(-\hat{\boldsymbol{n}},\pi)$. The sign ambiguity in the determination of $\hat{\boldsymbol{n}}$ in Case 3 cannot be resolved without examining the explicit form of the three dimensional proper rotation matrix $R(\hat{\boldsymbol{n}},\theta)$.

4. The eigenvalues and eigenvectors of improper rotation matrices in three dimensions

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,

$$\overline{R}(\hat{\boldsymbol{n}},\theta) \equiv R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}},\theta)\,. \tag{23}$$

Note that the improper rotation defined in eq. (23) 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,

$$\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(-\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}},0)\,, \tag{24}$$

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 $[\overline{R}(\hat{\boldsymbol{n}})]^2 = \mathbf{I}$, or equivalently, $[\overline{R}(\hat{\boldsymbol{n}})]^{-1} = \overline{R}(\hat{\boldsymbol{n}})$.

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

$$\overline{R}(\hat{\boldsymbol{n}},\pi) = R(\hat{\boldsymbol{n}},\pi)\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}},\pi) = -\mathbf{I}\,. \tag{25}$$

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

Two important differences between improper rotations in two and three dimensions are noteworthy. First, the inversion transformation, $-\mathbf{I}$, is a proper rotation in two dimensions, whereas in three dimensions it is an improper rotation. Second, in two dimensions, all improper rotation matrices satisfy $[\overline{R}(\theta)]^2=\mathbf{I}$ [cf. eq. (18)] and thus correspond to a pure reflection through a line that passes through the origin. In three dimensions, only some of the improper rotation matrices satisfy $[\overline{R}(\hat{\boldsymbol{n}},\theta)]^2=\mathbf{I}$ and therefore correspond to a pure reflection.

To learn more about the properties of a general three-dimensional improper rotation, we again consider the matrix representation $\overline{R}(\hat{\boldsymbol{n}},\theta)$ with respect to the standard basis $\mathcal{B}_s=\{\boldsymbol{i}\,,\,\boldsymbol{j}\,,\,\boldsymbol{k}\}$. We can define a new coordinate system in which the unit normal to the reflection plane $\hat{\boldsymbol{n}}$ points in the direction of the new z-axis; the corresponding new basis will be denoted by $\mathcal{B}'$. The matrix representation of the improper rotation with respect to $\mathcal{B}'$ is then given by

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

Using the formalism developed in the class handout, *Vector coordinates, matrix elements, changes of basis, and matrix diagonalization*, there exists an invertible matrix P such that

$$\overline{R}(\hat{\boldsymbol{n}},\theta)=P\overline{R}(\boldsymbol{k},\theta)P^{-1}\,. \tag{26}$$

The rest of the analysis mirrors the discussion of Section 3. It immediately follows that

$$\mathrm{Tr}\ \overline{R}(\hat{\boldsymbol{n}},\theta)=\mathrm{Tr}\ \overline{R}(\boldsymbol{k},\theta)=2\cos\theta-1\,, \tag{27}$$

after taking the trace of eq. (26). By convention, $0\leq\theta\leq\pi$, which implies that $\sin\theta\geq 0$. Hence, the rotation angle is uniquely determined by eq. (27) To identify $\hat{\boldsymbol{n}}$ (up to an overall sign), we observe that any vector that is parallel to $\hat{\boldsymbol{n}}$ (which points along the normal to the reflection plane) is inverted. This last statement can be expressed as an eigenvalue equation,

$$\overline{R}(\hat{\boldsymbol{n}},\theta)\hat{\boldsymbol{n}}=-\hat{\boldsymbol{n}}\,. \tag{28}$$

Thus, $\hat{\boldsymbol{n}}$ is an eigenvector of $\overline{R}(\hat{\boldsymbol{n}},\theta)$ corresponding to the eigenvalue -1. In particular, the eigenvalue -1 is nondegenerate for any $\theta\neq\pi$, in which case $\hat{\boldsymbol{n}}$ can be determined up to an overall sign by computing the corresponding normalized eigenvector of $\overline{R}(\hat{\boldsymbol{n}},\theta)$.

A simple proof of this result is given in Appendix A. Here, we shall establish this assertion by noting that the eigenvalues of any matrix are invariant with respect to a similarity transformation. Using eq. (26), it follows that the eigenvalues of $\overline{R}(\hat{\boldsymbol{n}},\theta)$ are identical to the eigenvalues of $\overline{R}(\boldsymbol{k},\theta)$. The latter can be obtained from the characteristic equation,

$$-(1+\lambda)\left[(\cos\theta-\lambda)^2+\sin^2\theta\right]=0\,,$$

which simplifies to:

$$(1+\lambda)(\lambda^2-2\lambda\cos\theta+1)=0\,.$$

Using the results of eqs. (5) and (6), it follows that the three eigenvalues of $\overline{R}(\boldsymbol{k},\theta)$ are given by,

$$\lambda_1=-1\,,\qquad \lambda_2=e^{i\theta}\,,\qquad \lambda_3=e^{-i\theta}\,,\qquad\quad \text{for}\;\;0\leq\theta\leq\pi\,.$$

There are three distinct cases:

Case 1:	$\theta=0$	$\lambda_1=\lambda_2=\lambda_3=-1\,,$	$\overline{R}(\hat{\boldsymbol{n}},\pi)=-\mathbf{I}\,,$
Case 2:	$\theta=\pi$	$\lambda_1=-1\,,\,\lambda_2=\lambda_3=1\,,$	$\overline{R}(\hat{\boldsymbol{n}},0)\equiv\overline{R}(\hat{\boldsymbol{n}})\,,$
Case 3:	$0<\theta<\pi$	$\lambda_1=-1,\lambda_2=e^{i\theta}\,,\,\lambda_3=e^{-i\theta}\,,$	$\overline{R}(\hat{\boldsymbol{n}},\theta)\,,$

where the corresponding improper rotation matrix is indicated for each of the three cases. Indeed, for $\theta\neq\pi$, the eigenvalue -1 is nondegenerate. Moreover, the other two eigenvalues are complex conjugates of each other, whose real part is equal to $\cos\theta$, which uniquely fixes the rotation angle in the convention where $0\leq\theta\leq\pi$.

Case 1 corresponds to inversion, $\vec{\boldsymbol{v}}\to-\vec{\boldsymbol{v}}$. Note that in this case, $\overline{R}(\hat{\boldsymbol{n}},\pi)=-\mathbf{I}$, independently of the direction of $\hat{\boldsymbol{n}}$.

Case 2 corresponds to a mirror reflection through a plane that is perpendicular to $\hat{\boldsymbol{n}}$ and passes through the origin. In this case, although the unit vector $\hat{\boldsymbol{n}}$ is determined only up to an overall sign by eq. (28), this sign ambiguity is immaterial in light of eq. (24). The doubly degenerate eigenvalue $+1$ in Case 2 is a consequence of the two linearly independent eigenvectors that span the reflection plane. In particular, any linear combination $\vec{\boldsymbol{v}}$ of these eigenvectors that lies in the reflection plane is unaffected by the reflection and thus satisfies $\overline{R}(\hat{\boldsymbol{n}})\vec{\boldsymbol{v}}=\vec{\boldsymbol{v}}$.

In the class handout entitled *Rotation Matrices in two, three and many dimensions*, the most general form of $\overline{R}(\hat{\boldsymbol{n}})$ was exhibited,

$$\overline{R}_{ij}(\hat{\boldsymbol{n}})=\begin{pmatrix}1-2n_1^2 & -2n_1n_2 & -2n_1n_3\\ -2n_1n_2 & 1-2n_2^2 & -2n_2n_3\\ -2n_1n_3 & -2n_2n_3 & 1-2n_3^2\end{pmatrix}\,. \tag{29}$$

As expected for a pure reflection, $\left[\overline{R}(\hat{\boldsymbol{n}})\right]^2=\mathbf{I}$, which can be verified by performing the matrix multiplication and using the fact that the unit vector $\hat{\boldsymbol{n}}$ satisfies $n_1^2+n_2^2+n_3^2=1$. One can also check that the following two vectors are eigenvectors of $\overline{R}_{ij}(\hat{\boldsymbol{n}})$, each with eigenvalue $+1$,

$$\begin{pmatrix}n_3\\0\\-n_1\end{pmatrix}\,,\qquad\begin{pmatrix}0\\n_3\\-n_2\end{pmatrix}\,.$$

Thus, any linear combination of the above two vectors lies in the reflection plane,

$$n_1 x + n_2 y + n_3 z = 0\,, \tag{30}$$

since the latter equation is satisfied by any linear combination of the two vectors above.

Finally, we note that the improper rotation matrices of Case 3 do not possess an eigenvalue of $+1$, since the vectors that lie in the reflection plane transform non-trivially under the proper rotation $R(\hat{\boldsymbol{n}},\theta)$. Moreover, the unit vector $\hat{\boldsymbol{n}}$ is determined only up to an overall sign by eq. (28). The sign ambiguity in the determination of $\hat{\boldsymbol{n}}$ in Case 3 cannot be resolved without examining the explicit form of the three dimensional improper rotation matrix $\overline{R}(\hat{\boldsymbol{n}},\theta)$.

The following example is instructive. First, we 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,

$$\begin{aligned}
n_1 &= \sin\theta_{\boldsymbol{n}}\cos\phi_{\boldsymbol{n}}\,,\\
n_2 &= \sin\theta_{\boldsymbol{n}}\sin\phi_{\boldsymbol{n}}\,,\\
n_3 &= \cos\theta_{\boldsymbol{n}}\,.
\end{aligned}$$

Consider an example in which $\theta_{\boldsymbol{n}} = \frac{1}{2}\pi$ and $\phi_{\boldsymbol{n}} = \frac{1}{2}(\pi+\theta)$. In this case, the unit vector $\hat{\boldsymbol{n}}$ is given by,

$$\hat{\boldsymbol{n}} = \bigl(-\sin(\tfrac{1}{2}\theta)\,,\,\cos(\tfrac{1}{2}\theta)\,,\,0\bigr)\,. \tag{31}$$

Plugging this result into eq. (29) yields,

$$\overline{R}_{ij}(\hat{\boldsymbol{n}}) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ \sin\theta & -\cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}\,. \tag{32}$$

We recognize this matrix as the generalization of eq. (7) to three dimensions, where the line of reflection in two dimensions has been promoted to a reflection plane in three dimensions. Employing eqs. (30) and (31), the equation for the reflection plane is given by

$$-x\sin\bigl(\tfrac{1}{2}\theta\bigr) + y\cos\bigl(\tfrac{1}{2}\theta\bigr) = 0\,, \tag{33}$$

which is equivalent to eq. (17). Indeed, eq. (33) is the equation for a plane whose intersection with the x–y plane is a straight line of slope $\tan\bigl(\frac{1}{2}\theta\bigr)$ that passes through the origin.

Appendix A: An explicit formula for the matrix $\boldsymbol{P}$ introduced in eq. (20)

Suppose we wish to determine the explicit form of the rotation matrix $R(\hat{\boldsymbol{n}},\theta)$. Here is one possible strategy. The matrix $R(\hat{\boldsymbol{n}},\theta)$ is specified with respect to the standard basis $\mathcal{B}_s = \{\boldsymbol{i}\,,\,\boldsymbol{j}\,,\,\boldsymbol{k}\}$. Given that the explicit form for $R(\hat{\boldsymbol{n}},\boldsymbol{k})$ is known [cf. eq. (19)] suggests that we should transform to a new orthonormal basis, $\mathcal{B}' = \{\boldsymbol{i}'\,,\,\boldsymbol{j}'\,,\,\boldsymbol{k}'\}$, in which new positive z-axis points in the direction of $\hat{\boldsymbol{n}}$. That is,

$$\boldsymbol{k}' = \hat{\boldsymbol{n}} \equiv (n_1, n_2, n_3)\,, \qquad \text{where}\quad n_1^2+n_2^2+n_3^2 = 1\,.$$

The new positive y-axis can be chosen to lie along

$$\boldsymbol{j}' = \left(\frac{-n_2}{\sqrt{n_1^2+n_2^2}}\,,\,\frac{n_1}{\sqrt{n_1^2+n_2^2}}\,,\,0\right)\,,$$

since by construction, $\boldsymbol{j}'$ is a unit vector orthogonal to $\boldsymbol{k}'$. We complete the new right-handed coordinate system by choosing:

$$\boldsymbol{i}' = \boldsymbol{j}'\times\boldsymbol{k}' = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & 0 \\ n_1 & n_2 & n_3 \end{vmatrix} = \left(\frac{n_3 n_1}{\sqrt{n_1^2+n_2^2}}\,,\,\frac{n_3 n_2}{\sqrt{n_1^2+n_2^2}}\,,\,-\sqrt{n_1^2+n_2^2}\right)\,.$$

Following the class handout entitled, *Vector coordinates, matrix elements, changes of basis, and matrix diagonalization*, we determine the matrix P whose matrix elements are defined by

$$\boldsymbol{b}'_j = \sum_{i=1}^{n} P_{ij}\hat{\boldsymbol{e}}_i\,,$$

where the $\hat{\boldsymbol{e}}_i = \{\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$ are the basis vectors of $\mathcal{B}_s$ and the $\boldsymbol{b}'_j$ are the basis vectors of $\mathcal{B}'$. The columns of P are the coefficients of the expansion of the new basis vectors in terms of the old basis vectors. Thus,

$$P = \begin{pmatrix} \dfrac{n_3 n_1}{\sqrt{n_1^2+n_2^2}} & \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & n_1 \\ \dfrac{n_3 n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & n_2 \\ -\sqrt{n_1^2+n_2^2} & 0 & n_3 \end{pmatrix}\,. \tag{34}$$

The inverse P^{-1} is easily computed since the columns of P are orthonormal, which implies that P is an orthogonal matrix, i.e. $P^{-1} = P^{\mathsf{T}}$.

According to eq. (16) of the class handout, *Vector coordinates, matrix elements, changes of basis and matrix diagonalization*,

$$[R]_{\mathcal{B}'} = P^{-1}\,[R]_{\mathcal{B}_s}\,P\,. \tag{35}$$

where $[R]_{\mathcal{B}_s}$ is the matrix R with respect to the standard basis, and $[R]_{\mathcal{B}'}$ is the matrix R with respect to the new basis (in which $\hat{\boldsymbol{n}}$ points along the new positive z-axis). In particular,

$$[R]_{\mathcal{B}} = R(\hat{\boldsymbol{n}},\theta)\,, \qquad [R]_{\mathcal{B}'} = R(\boldsymbol{k},\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}\,.$$

Hence, eq. (35) yields[2]

$$R(\hat{\boldsymbol{n}},\theta)=PR(\boldsymbol{k},\theta)P^{-1}\,, \tag{36}$$

where P is given by eq. (34) and $P^{-1}=P^{\mathsf{T}}$.

For ease of notation, we define

$$N_{12}\equiv\sqrt{n_1^2+n_2^2}\,. \tag{37}$$

Note that $N_{12}^2+n_3^2=1$, since $\hat{\boldsymbol{n}}$ is a unit vector. Writing out the matrices in eq. (36),

$$R(\hat{\boldsymbol{n}},\theta)=\begin{pmatrix} n_3n_1/N_{12} & -n_2/N_{12} & n_1\\ n_3n_2/N_{12} & n_1/N_{12} & n_2\\ -N_{12} & 0 & n_3\end{pmatrix}\begin{pmatrix}\cos\theta & -\sin\theta & 0\\ \sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix}\begin{pmatrix} n_3n_1/N_{12} & n_3n_2/N_{12} & -N_{12}\\ -n_2/N_{12} & n_1/N_{12} & 0\\ n_1 & n_2 & n_3\end{pmatrix}$$

$$=\begin{pmatrix} n_3n_1/N_{12} & -n_2/N_{12} & n_1\\ n_3n_2/N_{12} & n_1/N_{12} & n_2\\ -N_{12} & 0 & n_3\end{pmatrix}\begin{pmatrix}\frac{n_3n_1\cos\theta+n_2\sin\theta}{N_{12}} & \frac{n_3n_2\cos\theta-n_1\sin\theta}{N_{12}} & -N_{12}\cos\theta\\ \frac{n_3n_1\sin\theta-n_2\cos\theta}{N_{12}} & \frac{n_3n_2\sin\theta+n_1\cos\theta}{N_{12}} & -N_{12}\sin\theta\\ n_1 & n_2 & n_3\end{pmatrix}.$$

Using $N_{12}^2=n_1^2+n_2^2$ and $n_3^2=1-N_{12}^2$, the final matrix multiplication then yields,

$$R(\hat{\boldsymbol{n}},\theta)=\begin{pmatrix}\cos\theta+n_1^2(1-\cos\theta) & n_1n_2(1-\cos\theta)-n_3\sin\theta & n_1n_3(1-\cos\theta)+n_2\sin\theta\\ n_1n_2(1-\cos\theta)+n_3\sin\theta & \cos\theta+n_2^2(1-\cos\theta) & n_2n_3(1-\cos\theta)-n_1\sin\theta\\ n_1n_3(1-\cos\theta)-n_2\sin\theta & n_2n_3(1-\cos\theta)+n_1\sin\theta & \cos\theta+n_3^2(1-\cos\theta)\end{pmatrix} \tag{38}$$

which coincides with the result previously exhibited in the class handout entitled *Rotation matrices in two, three and many dimensions.*

Appendix B: The eigenvalues of a 3 × 3 orthogonal matrix[3]

Given any matrix A, the eigenvalues are the solutions to the characteristic equation,

$$\det\left(A-\lambda\mathbf{I}\right)=0\,. \tag{39}$$

Suppose that A is an $n\times n$ real orthogonal matrix. The eigenvalue equation for A and its complex conjugate transpose are given by:

$$A\boldsymbol{v}=\lambda\boldsymbol{v}\,,\qquad \boldsymbol{v}^{*\mathsf{T}}A^{\mathsf{T}}=\lambda^*\,\boldsymbol{v}^{*\mathsf{T}}\,.$$

Hence multiplying these two equations together yields

$$\lambda^*\lambda\,\boldsymbol{v}^{*\mathsf{T}}\boldsymbol{v}=\boldsymbol{v}^{*\mathsf{T}}A^{\mathsf{T}}A\,\boldsymbol{v}=\boldsymbol{v}^{*\mathsf{T}}\boldsymbol{v}\,, \tag{40}$$

[2] Eq. (36) is a special case of a more general result, $R(\hat{\boldsymbol{n}},\theta)=PR(\hat{\boldsymbol{n}}',\theta)P^{-1}$, where $\hat{\boldsymbol{n}}=P\hat{\boldsymbol{n}}'$.

[3] A nice reference to the results of this appendix can be found in L. Mirsky, *An Introduction to Linear Algebra* (Dover Publications, Inc., New York, 1982).

since an orthogonal matrix satisfies $A^{\mathsf{T}}A = \mathbf{I}$. Since eigenvectors must be nonzero, it follows that $\boldsymbol{v}^{*\mathsf{T}}\boldsymbol{v} \neq 0$. Hence, eq. (40) yields $|\lambda| = 1$. Thus, the eigenvalues of a real orthogonal matrix must be complex numbers of unit modulus. That is, $\lambda = e^{i\alpha}$ for some α in the interval $0 \leq \alpha < 2\pi$.

Consider the following product of matrices, where A satisfies $A^{\mathsf{T}}A = \mathbf{I}$,

$$A^{\mathsf{T}}(\mathbf{I} - A) = A^{\mathsf{T}} - \mathbf{I} = -(\mathbf{I} - A)^{\mathsf{T}}\,.$$

Taking the determinant of both sides of this equation, it follows that[4]

$$\det A \det(\mathbf{I} - A) = (-1)^n \det(\mathbf{I} - A)\,, \tag{41}$$

since for the $n \times n$ identity matrix, $\det(-\mathbf{I}) = (-1)^n$. For a proper odd-dimensional orthogonal matrix, we have $\det A = 1$ and $(-1)^n = -1$. Hence, eq. (41) yields[5]

$$\det(\mathbf{I} - A) = 0\,, \qquad \text{for any proper odd-dimensional orthogonal matrix } A. \tag{42}$$

Comparing with eq. (39), we conclude that $\lambda = 1$ is an eigenvalue of A. Since $\det A$ is the product of its three eigenvalues and each eigenvalue of A is a complex number of unit modulus,[6] it follows that the eigenvalues of any proper 3×3 orthogonal matrix must be 1, $e^{i\theta}$ and $e^{-i\theta}$ for some value of θ that lies in the interval $0 \leq \theta \leq \pi$.[7]

Next, we consider the following product of matrices, where A satisfies $A^{\mathsf{T}}A = \mathbf{I}$,

$$A^{\mathsf{T}}(\mathbf{I} + A) = A^{\mathsf{T}} + \mathbf{I} = (\mathbf{I} + A)^{\mathsf{T}}\,.$$

Taking the determinant of both sides of this equation, it follows that

$$\det A \det(\mathbf{I} + A) = \det(\mathbf{I} + A)\,, \tag{43}$$

For any improper orthogonal matrix, we have $\det A = -1$. Hence, eq. (43) yields

$$\det(\mathbf{I} + A) = 0\,, \qquad \text{for any improper orthogonal matrix } A.$$

Comparing with eq. (39), we conclude that $\lambda = -1$ is an eigenvalue of A. Since $\det A$ is the product of its three eigenvalues and each eigenvalue is a complex number of unit modulus, it follows that the eigenvalues of any improper 3×3 orthogonal matrix must be -1, $e^{i\theta}$ and $e^{-i\theta}$ for some value of θ that lies in the interval $0 \leq \theta \leq \pi$ (cf. footnote 7).

[4]Here, we make use of the well known properties of the determinant, namely $\det(AB) = \det A \det B$ and $\det(A^{\mathsf{T}}) = \det A$.

[5]Eq. (42) is also valid for any improper even-dimensional orthogonal matrix A since in this case $\det A = -1$ and $(-1)^n = 1$.

[6]If $A^{\mathsf{T}}A = \mathbf{I}$ and $A\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}$, then $\langle \vec{\boldsymbol{v}}, \vec{\boldsymbol{v}} \rangle = \langle A^{\mathsf{T}}A\,\vec{\boldsymbol{v}}\,,\, \vec{\boldsymbol{v}} \rangle = \langle A\vec{\boldsymbol{v}}, A\vec{\boldsymbol{v}} \rangle = \langle \lambda\vec{\boldsymbol{v}}, \lambda\vec{\boldsymbol{v}} \rangle = \lambda^*\lambda\langle \vec{\boldsymbol{v}}, \vec{\boldsymbol{v}} \rangle$, under the assumption that A is a real matrix. For more details on the property of the inner product, see Section 4 of the class handout entitled *Vector coordinates, matrix elements, changes of basis, and matrix diagonalization*. Hence, it follows that $\lambda^*\lambda = 1$ or equivalently $|\lambda| = 1$.

[7]There is no loss of generality in restricting the interval of the angle to satisfy $0 \leq \theta \leq \pi$. In particular, under $\theta \to 2\pi - \theta$, the two eigenvalues $e^{i\theta}$ and $e^{-i\theta}$ are simply interchanged.