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Projectors, Reflections, Rotations

We have already learned about reflections on a mirror plane spanned by two *Cartesian* unit vectors and rotations about one of the *Cartesian* axes. But what about reflections on arbitrary planes and rotations about arbitrary axes?

- Define the longitudinal and transverse projection operators P_L and P_T as well as the transverse rotation operator R_T (cross product matrix). Find their multiplication table.

Solution:

The longitudinal projection operator projects a given vector $\boldsymbol{x}$ onto a chosen vector $\boldsymbol{k}$. In index and matrix notation, this operator reads respectively

$$P_\mathrm{L}(\boldsymbol{k}) = \frac{\boldsymbol{k}\boldsymbol{k}^\intercal}{|\boldsymbol{k}|^2}\,, \qquad (P_\mathrm{L})_{ij}\,(\boldsymbol{k}) = \frac{k_i k_j}{|\boldsymbol{k}|^2}\,. \tag{1}$$

Since the sum of longitudinal and transverse components has to combine into the initial vector and hence

$$P_\mathrm{L} + P_\mathrm{T} = \mathbb{1}\,, \tag{2}$$

we can construct the transverse projection operator using the latter relation:

$$P_\mathrm{T}(\boldsymbol{k}) = \mathbb{1} - P_\mathrm{L}(\boldsymbol{k})\,, \quad (P_\mathrm{T})_{ij}\,(\boldsymbol{k}) = \delta_{ij} - \frac{k_i k_j}{|\boldsymbol{k}|^2}\,. \tag{3}$$

By rewriting this using the Graßmann formula, we further find for an application on a vector $\boldsymbol{x}$ the identity

$$P_\mathrm{T}(\boldsymbol{k})\,\boldsymbol{x} = \frac{|\boldsymbol{k}^2|\boldsymbol{x} - \boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{x})}{|\boldsymbol{k}|^2} = -\frac{\boldsymbol{k}\times(\boldsymbol{k}\times\boldsymbol{x})}{|\boldsymbol{k}|^2}\,. \tag{4}$$

The transverse rotation matrix (or cross product matrix a. k. a. skew-symmetric matrix) is given by

$$R_\mathrm{T}(\boldsymbol{k})\,\boldsymbol{x} := \frac{\boldsymbol{k}\times\boldsymbol{x}}{|\boldsymbol{k}|} = \frac{1}{|\boldsymbol{k}|}\begin{pmatrix} k_2x_3 - k_3x_2 \\ k_3x_1 - k_1x_3 \\ k_1x_2 - k_2x_1 \end{pmatrix} = \frac{1}{|\boldsymbol{k}|}\begin{pmatrix} 0 & -k_3 & k_2 \\ k_3 & 0 & -k_1 \\ -k_2 & k_1 & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}\,. \tag{5}$$

In case $\boldsymbol{k}$ is a unit vector, $\boldsymbol{n} = \boldsymbol{k}/|\boldsymbol{k}|$, these three operators simplify to

$$P_\mathrm{L}\,\boldsymbol{x} = \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x})\,, \quad P_\mathrm{T}\,\boldsymbol{x} = -\boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\,, \quad R_\mathrm{T}\,\boldsymbol{x} = \boldsymbol{n}\times\boldsymbol{x}\,. \tag{6}$$

Note: Do not confuse the rotation matrix R from the previous exercise with the projector R_T!

The three operators P_L, P_T and R_T form an algebra which is represented by the following multiplication table:

$\cdot$	P_L	P_T	R_T
P_L	P_L	0	0
P_T	0	P_T	R_T
R_T	0	R_T	$-P_\mathrm{T}$

$$\begin{aligned} &P_\mathrm{L}P_\mathrm{L}\,\boldsymbol{x} = \boldsymbol{n}[\boldsymbol{n}\cdot\boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x})] = \boldsymbol{n}[1(\boldsymbol{n}\cdot\boldsymbol{x})] = P_\mathrm{L}\,\boldsymbol{x} \\ &P_\mathrm{L}P_\mathrm{T} = P_\mathrm{L}(\mathbb{1} - P_\mathrm{L}) = P_\mathrm{L} - P_\mathrm{L} = 0 \\ &P_\mathrm{T} = -R_\mathrm{T}R_\mathrm{T} \\ &R_\mathrm{T}P_\mathrm{T}\,\boldsymbol{x} = R_\mathrm{T}(\mathbb{1} - P_\mathrm{L})\,\boldsymbol{x} = R_\mathrm{T}\,\boldsymbol{x} - \boldsymbol{n}\times[\boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x})] = R_\mathrm{T}\,\boldsymbol{x} \end{aligned} \tag{7}$$

A priori it is not obvious that this is a commutative algebra, which means you have to check e. g. $P_\mathrm{L}R_\mathrm{T}$ and $R_\mathrm{T}P_\mathrm{L}$ separately.

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- How could you tell if a given matrix describes a rotation, a reflection, an inversion or a combination of any of them?

Solution:

Mathematical Background

Rotations, inversions and reflections (i. e. proper and improper rotations) form the orthogonal group in three dimensions, $O(3)$. Its elements can be represented by orthogonal matrices whose eigenvalues are of the form $\lambda = \mathrm{e}^{\mathrm{i}\varphi}$, i. e. the only possible real ones are $\lambda_{\mathbb{R}} = \pm 1$.

Proof: Applying a matrix to one of its eigenvectors will simply scale this vector by the corresponding eigenvalue,

$$A\boldsymbol{v} = \lambda \boldsymbol{v}\,. \tag{8}$$

Now consider the norm of the eigenvector,

$$\|A\boldsymbol{v}\| = \|\lambda \boldsymbol{v}\|\,, \tag{9}$$

and recall that orthogonal matrices Q with $Q^\intercal = Q^{-1}$ preserve the Euclidean norm,

$$\|Q\boldsymbol{v}\| \overset{\text{def.}}{=} \sqrt{(Q\boldsymbol{v})^\intercal (Q\boldsymbol{v})} \overset{\text{trans.}}{=} \sqrt{\boldsymbol{v}^\intercal (Q^\intercal Q)\boldsymbol{v}} \overset{\text{orth.}}{=} \sqrt{\boldsymbol{v}^\intercal \boldsymbol{v}} \overset{\text{def.}}{=} \|\boldsymbol{v}\|\,, \tag{10}$$

such that for $A \in O(3)$

$$\|\boldsymbol{v}\| \overset{(10)}{=} \|A\boldsymbol{v}\| \overset{(8)}{=} \|\lambda \boldsymbol{v}\| = |\lambda|\|\boldsymbol{v}\|\,. \tag{11}$$

Since $\boldsymbol{v} \neq \boldsymbol{0}$ by definition of eigenvectors, it follows that

$$|\lambda| = 1 \quad \Rightarrow \quad \lambda = \mathrm{e}^{\mathrm{i}\varphi}\,, \varphi \in \mathbb{R}\,, \tag{12}$$

i. e. all possible eigenvalues are located on the unit circle in the complex plane. ∎

Eigenvectors of orthogonal matrices corresponding to distinct eigenvalues are mutually orthogonal. For eigenvalues with algebraic multiplicity > 1, a set of eigenvectors can be constructed in a way that they are mutually orthogonal as well, although for our purpose the less restrictive linear independence would be already sufficient, which is automatically fullfilled.

Proof: We begin with the eigenvalue equation for two distinct eigenvalues $\lambda_1 \neq \lambda_2$ of a real orthogonal matrix $A \in \mathrm{O}(3, \mathbb{R})$ with $A^\dagger := (A^\intercal)^* \overset{\text{real}}{=} A^\intercal \overset{\text{orth.}}{=} A^{-1}$,

$$A\boldsymbol{v_1} = \lambda_1 \boldsymbol{v_1}\,, \quad A\boldsymbol{v_2} = \lambda_2 \boldsymbol{v_2}\,. \tag{13}$$

Plugging the LHS of each equation into an inner product (complex vector space!) yields

$$\langle A\boldsymbol{v}_1, A\boldsymbol{v}_2\rangle = \langle \boldsymbol{v}_1, (A^\dagger A)\,\boldsymbol{v}_2\rangle = \langle \boldsymbol{v}_1, \boldsymbol{v}_2\rangle\,. \tag{14}$$

On the other hand we know because of sesquilinearity of the inner product

$$\langle A\boldsymbol{v}_1, A\boldsymbol{v}_2\rangle = \langle \lambda_1\boldsymbol{v}_1, \lambda_2\boldsymbol{v}_2\rangle = \lambda_1\lambda_2^* \langle \boldsymbol{v}_1, \boldsymbol{v}_2\rangle\,. \tag{15}$$

Equating both expressions gives the following condition

$$(1 - \lambda_1\lambda_2^*)\langle \boldsymbol{v}_1, \boldsymbol{v}_2\rangle = 0\,, \tag{16}$$

which can only be true in two cases. Apparently, the first option leads to a contradiction since we required $\lambda_1 \neq \lambda_2$ in the beginning:

$$1 \overset{!}{=} \lambda_1\lambda_2^* = |\lambda_1||\lambda_2|\, e^{\mathrm{i}\varphi_1}\, e^{-\mathrm{i}\varphi_2} \overset{(12)}{=} e^{\mathrm{i}(\varphi_1 - \varphi_2)} \quad \Rightarrow \quad \varphi_1 = \varphi_2 \quad \Rightarrow \quad \lambda_1 = \lambda_2 \quad ↯ \tag{17}$$

Hence we find for the remaining second option

$$\langle \boldsymbol{v}_1, \boldsymbol{v}_2\rangle = 0\,, \tag{18}$$

i. e. any pair of eigenvectors with different eigenvalues must be orthogonal. ∎

In the upcoming tasks we will show by example that the different symmetry operations can be identified by the following characteristic properties of their representing matrices:

1. Inversions can be identified directly, because $I = -\mathbb{1}$.
2. Pure rotations have determinant $+1$ and a single real eigenvalue $+1$, improper rotations like roto-reflections and roto-inversions have -1 for both.
3. Pure reflections (without rotations) have three real eigenvalues. The eigenvector corresponding to $\lambda_1 = -1$ is the plane normal vector, whereas the two eigenvectors corresponding to $\lambda_{2/3} = 1$ span the mirror plane.
4. Any matrix with a rotation component has only one real eigenvalue $\lambda_1 = \pm 1$ (depending on the presence of a mirror component), and two complex conjugated eigenvalues $\lambda_{2/3} = \mathrm{e}^{\pm \mathrm{i}\varphi}$ with corresponding complex conjugated eigenvectors $\boldsymbol{v}_2 = \boldsymbol{v}_3^*$. By constructing two new *real* vectors via
$$\boldsymbol{w}_1 = \frac{\boldsymbol{v}_2 + \boldsymbol{v}_3}{\sqrt{2}}, \quad \boldsymbol{w}_2 = \frac{\boldsymbol{v}_2 - \boldsymbol{v}_3}{\sqrt{2}\mathrm{i}}, \tag{19}$$
we can span the plane of rotation.
5. In general, you cannot tell any intermediate steps like multiple rotations, reflections or arbitrary combinations, but only the resulting or effective symmetry operation. This is because there is no unique way of reaching a specific configuration.

- Find the matrix for reflections on arbitrary planes (containing the origin) with a normal unit vector $\boldsymbol{n}$. For a given reflection matrix, find the corresponding plane.

Solution:

In order to calclulate the matrix corresponding to a reflection on a plane that contains the origin, we may use the definition of the Householder matrix,
$$H = \mathbb{1} - 2\boldsymbol{n}\boldsymbol{n}^\intercal = \mathbb{1} - 2P_\mathrm{L} = P_\mathrm{T} - P_\mathrm{L}, \tag{20}$$
which essentially subtracts twice the projection of a vector onto the plane normal. For testing, we apply some example matrices to vectors whose reflection can easily be verified.

Fun fact: The Householder matrix or transformation is an important concept in numerical mathematics, namely for QR decomposition, as well as in video game development.

Examples:

1. Normal vector $\boldsymbol{n_1} = (1, 0, 0)^\intercal$

Householder matrix:
$$H_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - 2\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{21}$$

Test for vector in xy-plane and vector parallel to reflection plane:
$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \quad \checkmark \tag{22}$$
$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \quad \checkmark \tag{23}$$

2. Normal vector $\boldsymbol{n}_2 = 1/\sqrt{3}\,(1,1,1)^\intercal$

   Householder matrix:

$$H_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{2}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 1/3 & -2/3 & -2/3 \\ -2/3 & 1/3 & -2/3 \\ -2/3 & -2/3 & 1/3 \end{pmatrix} \tag{24}$$

   Test for vectors $\perp$ and $\parallel$ to reflection plane:

$$\begin{pmatrix} 1/3 & -2/3 & -2/3 \\ -2/3 & 1/3 & -2/3 \\ -2/3 & -2/3 & 1/3 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix} \quad \checkmark \tag{25}$$

$$\begin{pmatrix} 1/3 & -2/3 & -2/3 \\ -2/3 & 1/3 & -2/3 \\ -2/3 & -2/3 & 1/3 \end{pmatrix}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \quad \checkmark \tag{26}$$

Inverse Problem

For odd dimensions like $\mathbb{R}^3$ where 3x3 matrices have at least 1 real eigenvalue (complex eigenvalues always emerge in conjugated pairs), a reflection matrix has to possess an eigenvector $\boldsymbol{v}_\mathrm{n}$ such that

$$H\boldsymbol{v}_\mathrm{n} = -\boldsymbol{v}_\mathrm{n}\,, \quad \boldsymbol{v}_\mathrm{n} \parallel \boldsymbol{n}\,. \tag{27}$$

In other words, we can find an eigenvector of H whose entries will all change sign after applying the reflection matrix to it. Consequently, this vector has to be parallel to the plane normal $\boldsymbol{n}$. Thus, the problem of finding the plane corresponding to a reflection matrix is equal to finding the eigenvector corresponding to the eigenvalue $\lambda = -1$.

Examples:[1]

$$H_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \left|\begin{array}{ll} \lambda_1 = -1\,, & \boldsymbol{v}_1 = (1,0,0)^\intercal \\ \lambda_2 = 1\,, & \boldsymbol{v}_2 = (0,1,0)^\intercal \\ \lambda_3 = 1\,, & \boldsymbol{v}_3 = (0,0,1)^\intercal \end{array}\right. \quad \Rightarrow \quad \boldsymbol{v}_1 \parallel \boldsymbol{n}_1 \ \checkmark \tag{28}$$

$$H_2 = \begin{pmatrix} 1/3 & -2/3 & -2/3 \\ -2/3 & 1/3 & -2/3 \\ -2/3 & -2/3 & 1/3 \end{pmatrix}, \quad \left|\begin{array}{ll} \lambda_1 = -1\,, & \boldsymbol{v}_1 = (1,1,1)^\intercal \\ \lambda_2 = 1\,, & \boldsymbol{v}_2 = (-1,1,0)^\intercal \\ \lambda_3 = 1\,, & \boldsymbol{v}_3 = (-1,0,1)^\intercal \end{array}\right. \quad \Rightarrow \quad \boldsymbol{v}_1 \parallel \boldsymbol{n}_2 \ \checkmark \tag{29}$$

The reflection plane itself could technically be described by one of the plane equations, e. g.

$$\boldsymbol{x}\cdot\boldsymbol{n} = 0 \quad \Leftrightarrow \quad n_1x + n_2y + n_3z = 0\,, \quad (n_1,n_2,n_3)^\intercal = \boldsymbol{n}\,. \tag{30}$$

[1] Note, that when having algebraic multiplicity $\mu_i > 1$ for any eigenvalue λ_i of matrix A, then the associated eigenspace $\mathrm{Eig}_A(\lambda_i) = \mathcal{N}(A - \lambda_i\mathbb{1})$ can have at most dimension μ_i. In case of H_2 we find $H_2 - \lambda_{2/3}\mathbb{1} = -2/3J_3$ (J_3 is 3x3 matrix of ones) and consequently the underconstrained equation $x_1 + x_2 + x_3 = 0$. A general vector from this eigenspace reads

$$\boldsymbol{v} = \begin{pmatrix} -x_2 - x_3 \\ x_2 \\ x_3 \end{pmatrix} = x_2\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} + x_3\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

In order to find a suitable and convenient basis of this subspace, we simply set $x_2 = 0$ and $x_3 = 0$, respectively. The two resulting vectors are automatically orthogonal to each other and span $\mathrm{Eig}_{H_2}(\lambda_2)$.

- Find the matrix of a rotation about an arbitrary axis (crossing the origin). For a given rotation matrix, find the corresponding rotation axis and angle.

  Solution:

  A general counter-clockwise rotation of a vector $\boldsymbol{x}$ by angle φ about an arbitrary axis $\boldsymbol{n}$ (with $\boldsymbol{n} \cdot \boldsymbol{n} = 1$) is given by the Rodrigues formula

$$R(\varphi\boldsymbol{n})\boldsymbol{x} = \boldsymbol{n}(\boldsymbol{n} \cdot \boldsymbol{x}) + (\boldsymbol{n} \times \boldsymbol{x})\sin\varphi - \boldsymbol{n} \times (\boldsymbol{n} \times \boldsymbol{x})\cos\varphi \tag{31}$$

$$= \boldsymbol{n}(\boldsymbol{n} \cdot \boldsymbol{x})(1 - \cos\varphi) + (\boldsymbol{n} \times \boldsymbol{x})\sin\varphi + \boldsymbol{x}\cos\varphi\,. \tag{32}$$

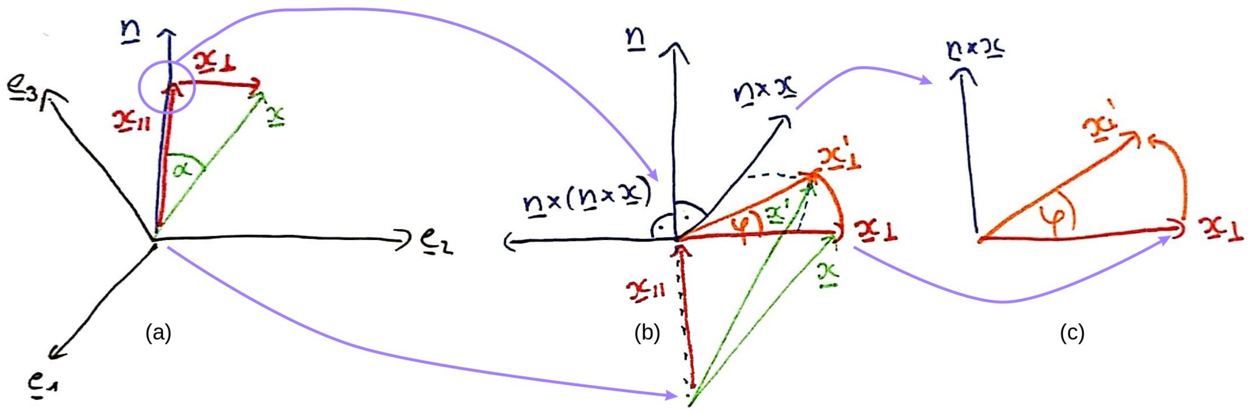

Figure 1: (a) Decomposition of $\boldsymbol{x}$ into $\boldsymbol{x}_\parallel = P_\mathrm{L}\boldsymbol{x}$ and $\boldsymbol{x}_\perp = P_\mathrm{T}\boldsymbol{x}$, (b) zoom into a new Cartesian system where $\boldsymbol{x}_\perp$ is rotated about $\boldsymbol{n}$ by φ to $\boldsymbol{x}'_\perp = R(\varphi\boldsymbol{n})\boldsymbol{x}_\perp$, (c) 2D view of the transverse plane with non-normal basis vectors $\boldsymbol{x}_\perp = -\boldsymbol{n} \times (\boldsymbol{n} \cdot \boldsymbol{x})$ and $\boldsymbol{n} \times \boldsymbol{x}$.

Heuristic derivation

We want to verify the composing terms of the Rodrigues formula using elementary geometry:

1. First, we decompose the initial vector $\boldsymbol{x}$ into its longitudinal and transverse parts (with respect to the normal vector $\boldsymbol{n}$) using the two projection operators,

$$\boldsymbol{x}_\parallel \coloneqq P_\mathrm{L}(\boldsymbol{n})\boldsymbol{x}, \quad \boldsymbol{x}_\perp \coloneqq P_\mathrm{T}(\boldsymbol{n})\boldsymbol{x}, \quad \boldsymbol{x}_\parallel + \boldsymbol{x}_\perp = \boldsymbol{x}\,. \tag{33}$$

   You can find these two components in Fig. 1 (a) emphasized in red.

2. Next, we zoom into the transverse plane corresponding to the rotation axis $\boldsymbol{n}$. How can we find the spanning vectors? By construction, $\boldsymbol{x}_\perp$ is orthogonal to $\boldsymbol{n}$, because it has been built using the *transverse* projection operator. Thus, it already lies within the transverse plane. So we only need one other vector that is orthogonal to $\boldsymbol{n}$ but may not be parallel to $\boldsymbol{x}_\perp$. Let's choose $\boldsymbol{n} \times \boldsymbol{x}$.

   Note, that we explicitly did not choose $\boldsymbol{n} \times \boldsymbol{x}_\perp$, because we need expressions in terms of $\boldsymbol{n}$ and $\boldsymbol{x}$ as will become clear later. However, the resulting vectors in both cases point in the same direction, but have different magnitudes.

3. By using the identity from Eq. (4), we further find

$$\boldsymbol{x}_\perp = -\boldsymbol{n} \times (\boldsymbol{n} \times \boldsymbol{x}) \quad \Rightarrow \quad |\boldsymbol{x}_\perp| = |\boldsymbol{n} \times (\boldsymbol{n} \times \boldsymbol{x})|\,. \tag{34}$$

4. Up to now, we only have (1) decomposed $\boldsymbol{x}$ and (2) created a new Cartesian system with origin at the intersection of $\boldsymbol{x}_\parallel$ and $\boldsymbol{x}_\perp$ (see Fig. 1 (a) and (b)). What's left is to rotate

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$\boldsymbol{x}_\perp$ within the transverse plane by φ. This is achieved just like in the 2D case where

$$\boldsymbol{x}' = r \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} = \boldsymbol{e}_1\, r\cos\varphi + \boldsymbol{e}_2\, r\sin\varphi\,, \tag{35}$$

with the only difference that we have more complex and especially non-normal base vectors (see Fig. 1 (c)):

$$\boldsymbol{x}'_\perp = |\boldsymbol{x}_\perp| \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix} = |\boldsymbol{x}_\perp| \left(\frac{\boldsymbol{x}_\perp}{|\boldsymbol{x}_\perp|}\,\cos\varphi + \frac{\boldsymbol{n}\times\boldsymbol{x}}{|\boldsymbol{n}\times\boldsymbol{x}|}\,\sin\varphi \right)\,. \tag{36}$$

In the first term we can immediately cancel $|\boldsymbol{x}_\perp|$. In the second term it is however not so obvious, but we can make use of Eq. (4) again:

$$|\boldsymbol{x}_\perp| = |\boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})| = |\boldsymbol{n}||\boldsymbol{n}\times\boldsymbol{x}|\sin\angle(\boldsymbol{n},\boldsymbol{n}\times\boldsymbol{x}) = |\boldsymbol{n}\times\boldsymbol{x}|\,. \tag{37}$$

Thus, we end up with

$$\boldsymbol{x}'_\perp = -\boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\cos\varphi + (\boldsymbol{n}\times\boldsymbol{x})\sin\varphi\,. \tag{38}$$

5. What about the longitudinal part $\boldsymbol{x}'_\parallel$? Since it is parallel to $\boldsymbol{n}$ by construction, it won't change during a rotation about $\boldsymbol{n}$, so $\boldsymbol{x}'_\parallel = \boldsymbol{x}_\parallel = \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x})$.
6. Finally, we have to add up the rotated transverse and the unchanged longitudinal components in order to construct the transformed vector $\boldsymbol{x}'$:

$$\begin{aligned}
\boldsymbol{x}' \overset{\text{Definition}}{=} R\boldsymbol{x} &\overset{\text{Decomposition}}{=} R(\boldsymbol{x}_\parallel + \boldsymbol{x}_\perp) &(39)\\
&\overset{\text{Linearity}}{=} R(\boldsymbol{x}_\parallel) + R(\boldsymbol{x}_\perp) &(40)\\
&\overset{\text{Definition}}{=} \boldsymbol{x}'_\parallel + \boldsymbol{x}'_\perp &(41)\\
&\overset{\text{Inserting}}{=} \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) + (\boldsymbol{n}\times\boldsymbol{x})\sin\varphi - \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\cos\varphi\,. &(42)
\end{aligned}$$

This is exactly the Rodrigues formula as introduced in Eq. (31).

Transformation Matrix

By applying the Graßmann formula,

$$\boldsymbol{a}\times(\boldsymbol{b}\times\boldsymbol{c}) = \boldsymbol{b}(\boldsymbol{a}\cdot\boldsymbol{c}) - \boldsymbol{c}(\boldsymbol{a}\cdot\boldsymbol{b})\,, \tag{43}$$

the other way around on Eq. (31), we find

$$\begin{aligned}
R(\varphi\boldsymbol{n})\boldsymbol{x} &= \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{x}) && + (\boldsymbol{n}\times\boldsymbol{x})\sin\varphi - \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\cos\varphi &(44)\\
&= \boldsymbol{x}(\boldsymbol{n}\cdot\boldsymbol{n}) + \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x}) && + (\boldsymbol{n}\times\boldsymbol{x})\sin\varphi - \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})\cos\varphi &(45)\\
&= \boldsymbol{x} \quad + \boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{x})(1-\cos\varphi) && + (\boldsymbol{n}\times\boldsymbol{x})\sin\varphi &(46)\\
&= \mathbb{1}\boldsymbol{x} \quad + R_\mathrm{T}(\boldsymbol{n})\left(R_\mathrm{T}(\boldsymbol{n})\boldsymbol{x}\right)(1-\cos\varphi) && + R_\mathrm{T}(\boldsymbol{n})\boldsymbol{x}\sin\varphi &(47)
\end{aligned}$$

The corresponding transformation matrices of Eq. (31), (32) and (47),

$$\begin{aligned}
R &= P_\mathrm{L} + R_\mathrm{T}\sin\varphi + P_\mathrm{T}\cos\varphi &(48)\\
&= P_\mathrm{L}(1-\cos\varphi) + R_\mathrm{T}\sin\varphi + \mathbb{1}\cos\varphi &(49)\\
&= \mathbb{1} + R_\mathrm{T}\sin\varphi + R_\mathrm{T}^2(1-\cos\varphi)\,, &(50)
\end{aligned}$$

can be found by simply reading off the definitions of P_L, P_T and R_T.

Examples:

1. Rotation by angle φ about normal vector $\boldsymbol{n}_3 = \boldsymbol{e}_z$

$$R(\varphi \boldsymbol{e}_z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \sin\varphi \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + (1-\cos\varphi) \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{51}$$

$$= \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \checkmark \tag{52}$$

2. Rotation by angle $\varphi = 2\pi/3 \mathrel{\hat{=}} 120°$ about space diagonal $\boldsymbol{n}_4 = 1/\sqrt{3}\,(1,1,1)^\intercal$

$$R(\varphi \boldsymbol{n}_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \frac{\sin\varphi}{\sqrt{3}} \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix} + \frac{(1-\cos\varphi)}{3} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \tag{53}$$

$$= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{54}$$

$\varphi \rightarrow$	0	$30° \mathrel{\hat{=}} \frac{\pi}{6}$	$45° \mathrel{\hat{=}} \frac{\pi}{4}$	$60° \mathrel{\hat{=}} \frac{\pi}{3}$	$90° \mathrel{\hat{=}} \frac{\pi}{2}$	$120° \mathrel{\hat{=}} \frac{2\pi}{3}$
$\sin\varphi$	0	$\frac{\sqrt{1}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{2}$	1	$\frac{\sqrt{3}}{2}$
$\cos\varphi$	1	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{1}}{2}$	0	$-\frac{1}{2}$
$\tan\varphi$	0	$\frac{\sqrt{3}}{3}$	1	$\frac{3}{\sqrt{3}}$	0	$-\frac{3}{\sqrt{3}}$

$$\text{Check:} \quad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \checkmark, \qquad \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \checkmark \tag{55}$$

Inverse Problem

Quite similar to the reflection case, a rotation matrix has to posess an eigenvector $\boldsymbol{v}_\mathrm{n}$ such that

$$R(\varphi \boldsymbol{n})\,\boldsymbol{v}_\mathrm{n} = \boldsymbol{v}_\mathrm{n}\,, \quad \boldsymbol{v}_\mathrm{n} \parallel \boldsymbol{n}\,, \tag{56}$$

i. e. every point on the rotation axis stays unchanged during this symmetry operation. Thus the problem of finding the rotation axis from a given matrix reduces to finding the eigenvector corresponding to the eigenvalue $+1$.

Examples:

$$R(\varphi \boldsymbol{e}_z) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \left| \begin{array}{ll} \lambda_1 = 1\,, & \boldsymbol{v}_1 = (0,0,1)^\intercal \\ \lambda_2 = \mathrm{e}^{\mathrm{i}\varphi}\,, & \boldsymbol{v}_2 = (-\mathrm{i},1,0)^\intercal \\ \lambda_3 = \mathrm{e}^{-\mathrm{i}\varphi}\,, & \boldsymbol{v}_3 = (\mathrm{i},1,0)^\intercal \end{array} \right. \quad \Rightarrow \quad \boldsymbol{v}_1 \parallel \boldsymbol{n}_3 \ \checkmark \tag{57}$$

$$R(\varphi \boldsymbol{n}_4) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \left| \begin{array}{ll} \lambda_1 = 1\,, & \boldsymbol{v}_1 = (1,1,1)^\intercal \\ \lambda_2 = \frac{-1-\sqrt{3}\mathrm{i}}{2}\,, & \boldsymbol{v}_2 = \text{not so easy} \\ \lambda_3 = \frac{-1+\sqrt{3}\mathrm{i}}{2}\,, & \boldsymbol{v}_3 = \text{not so easy} \end{array} \right. \quad \Rightarrow \quad \boldsymbol{v}_1 \parallel \boldsymbol{n}_4 \ \checkmark \tag{58}$$

Note: Although $R(\varphi \boldsymbol{e}_z)$ looks rather simple, calculating its eigenvectors is quite intricate[2].

For finding the rotation angle, we could either choose an arbitrary vector orthogonal to the rotation axis $\boldsymbol{x} \cdot \boldsymbol{n} = 0$ and find the angle between the vector before and after the rotation,

$$\varphi = \arccos\left(\frac{\boldsymbol{x} \cdot R\boldsymbol{x}}{|\boldsymbol{x}||R\boldsymbol{x}|}\right) , \tag{59}$$

or, more easily, we can calculate the trace of the rotation matrix via Eq. (50),

$$\begin{aligned} \mathrm{Tr}(R) &= \mathrm{Tr}(\mathbb{1}) + \sin\varphi\,\mathrm{Tr}(R_\mathrm{T}) + (1-\cos\varphi)\,\mathrm{Tr}(R_\mathrm{T}^2) && (60)\\ &= 1 + 2\cos\varphi\,, && (61) \end{aligned}$$

where we have used

$$\mathrm{Tr}(\alpha A + \beta B) = \alpha\,\mathrm{Tr}(A) + \beta\,\mathrm{Tr}(B)\,, \tag{62}$$

as well as $\mathrm{Tr}(\mathbb{1}) = 3$, $\mathrm{Tr}(R_\mathrm{T}) = 0$ and

$$\mathrm{Tr}(R_\mathrm{T}^2) = \mathrm{Tr}\begin{pmatrix} -n_2^2 - n_3^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & -n_1^2 - n_3^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & -n_1^2 - n_2^2 \end{pmatrix} \tag{63}$$

$$\begin{aligned} &= -2(n_1^2 + n_2^2 + n_3^2) = -2(\boldsymbol{n} \cdot \boldsymbol{n}) && (64)\\ &= -2\,. && (65) \end{aligned}$$

Note, that the sign of φ has to be chosen according to the direction ($\pm$) of the rotation axis.

Examples:

$$\mathrm{Tr}\begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} = 1 + 2\cos\varphi \quad \checkmark \tag{66}$$

$$\mathrm{Tr}\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = 0 \stackrel{!}{=} 1 + 2\cos\varphi \qquad \Rightarrow \qquad \varphi_{\pm \boldsymbol{n}_4} = \pm\frac{2}{3}\pi \mathrel{\hat{=}} \pm 120° \quad \checkmark \tag{67}$$

[2]For the eigenvalues of $R(\varphi \boldsymbol{e}_z)$ we find

$$(1-\lambda)[(\cos\varphi - \lambda)^2 + \sin^2\varphi)] = 0 \quad \xRightarrow[\sin^2+\cos^2=1]{\lambda_1=1} \quad \lambda^2 - 2\lambda\cos\varphi + 1 = 0 \quad \Longrightarrow \quad \lambda_{2/3} = \cos\varphi \pm \mathrm{i}\sin\varphi = \mathrm{e}^{\pm\mathrm{i}\varphi}.$$

The associated system of equations for calculating the components of eigenvector $\boldsymbol{v}_1 = (x, y, z)^\intercal$ is $0z = 0$ and

$$\text{(I)} \begin{array}{l} (\cos\varphi - 1)x - \sin\varphi\, y = 0 \\ \sin\varphi\, x + (\cos\varphi - 1)y = 0 \end{array} \quad \xRightarrow{\varphi\neq 0} \quad \text{(II)} \begin{array}{l} x = \frac{\sin\varphi}{\cos\varphi - 1}\, y \\ x = -\frac{\cos\varphi - 1}{\sin\varphi}\, y \end{array} \quad \xRightarrow{y\neq 0} \quad \text{(III)}\ \sin^2\varphi + (\cos\varphi - 1)^2 = 0 \quad \lightning$$

Apparently, z can be chosen arbitrarily. For x and y, we can check the case $\varphi = 0$ directly in (I). Here, any real vector is a valid eigenvector and consequently a rotation axis, since nothing will be rotated in the first place.
For non-zero φ, (III) leads to a contradiction: Both terms, $\sin^2\varphi$ and $(\cos\varphi - 1)^2$, are non-negative, hence must be zero simultaneously, which is only possible for $\varphi = k\pi$ and $\varphi = 2k\pi$ with $k \in \mathbb{Z}$, respectively. Combining both conditions and restricting φ to the interval $[0, 2\pi)$ yields $\varphi = 0$ which we excluded explicitly. $\lightning$
This renders $y = 0$ and via (I) also $x = 0$, together with an arbitrary z the only non-trivial solution: $\boldsymbol{v}_1 = (0, 0, z)^\intercal$

- **Bonus:** Perform a decomposition of the rotation by $2\pi/3$ about the space diagonal into a product of fundamental rotations R_{z-x-z} and R_{z-y-x}. Why is the first decomposition usually preferred, even if it does not rotate at least once about each of the three Cartesian axes?
  Solution:
  We simply compare the entries of the given rotation matrix $R(\varphi \boldsymbol{n})$ with the ones from R_{z-x-z} and R_{z-y-x} (check **Notes** section at the end of the document for details).
  Examples:
  1. For a rotation about $[1,1,1]^\intercal$ by 120° we find for R_{z-x-z} the following *unique* Euler angles:
  $$\begin{aligned} &\text{33-component:} && \cos(\beta) &&= 0 && \rightarrow && \beta = \frac{\pi}{2} && (68)\\ &\text{32-component:} && \cos(\alpha)\sin(\beta) = \cos(\alpha) &&= 1 && \rightarrow && \alpha = 0 && (69)\\ &\text{13-component:} && \sin(\beta)\sin(\gamma) = \sin(\gamma) &&= 1 && \rightarrow && \gamma = \frac{\pi}{2} && (70)\end{aligned}$$
  $$\text{Test:} \quad R_{z-x-z}\left(\alpha = 0, \beta = \frac{\pi}{2}, \gamma = \frac{\pi}{2}\right) = R\left(\frac{2\pi}{3}\boldsymbol{n}_4\right). \quad \checkmark \tag{71}$$
  Similarly, we find for R_{z-y-x} the following *two* valid sets of angles:
  $$\begin{aligned} &\text{31-component:} && -\sin(\beta) &&= 0 && \rightarrow && \beta_1 = 0, \quad \beta_2 = \pi && (72)\\ &\text{32-component:} && \sin(\alpha)\cos(\beta) = \pm\sin(\alpha) &&= 1 && \rightarrow && \alpha_1 = \frac{\pi}{2}, \quad \alpha_2 = \frac{3\pi}{2} && (73)\\ &\text{11-component:} && \cos(\beta)\cos(\gamma) = \pm\cos(\gamma) &&= 0 && \rightarrow && \gamma_1 = \frac{\pi}{2}, \quad \gamma_2 = \frac{3\pi}{2} && (74)\end{aligned}$$
  $$\text{Test:}\; R_{z-y-x}(\alpha_1,\beta_1,\gamma_1) = R\left(\frac{2\pi}{3}\boldsymbol{n}_4\right) \checkmark, \quad R_{z-y-x}(\alpha_2,\beta_2,\gamma_2) = R\left(\frac{2\pi}{3}\boldsymbol{n}_4\right) \checkmark \tag{75}$$
  Note: Not every combination you find using only 3 matrix components may yield the desired rotation matrix. The set of angles have to fullfill all the other equations as well. You can test this best by writing a small computer program that will print the resulting matrix for a given set. In case the original rotation matrix is retained, the set is valid, but in case any of the components turn out to be different from the input matrix, the set is no solution.
  2. For a rotation about the $\boldsymbol{e}_z$ axis by 180° we find for R_{z-x-z} the following Euler angles: From the 33-component we can deduce $\beta = 0$ and since $\sin(\beta) = 0$, all remaining elements of the 3rd row and column yield the equation $0 = 0$ and cannot be used further.
  $$\begin{aligned} &11/22: && \cos(\alpha)\cos(\gamma) - \sin(\alpha)\sin(\gamma) = \cos(\alpha+\gamma) = -1 && \rightarrow && \alpha + \gamma = \pi + 2\pi k && (76)\\ &12/21: && \cos(\alpha)\sin(\gamma) + \sin(\alpha)\cos(\gamma) = \sin(\alpha+\gamma) = 0 && \rightarrow && \alpha+\gamma = \pi k, k \in \mathbb{Z} && (77)\end{aligned}$$
  Since the 11/22 result is more restrictive, we obtain only one solution: $\alpha + \gamma = \pi$, whereas $\alpha + \gamma = 0$ is no solution.
  $$\text{Test:}\; R_{z-x-z}(42, 0, \pi - 42) = \mathrm{diag}(-1,-1,1) = R(\pi \boldsymbol{e}_z) \quad \checkmark \tag{78}$$

  Especially in vehicle and aircraft engineering, there are certain conventions like the Z-X-Z multiplication order which are preferred over the Z-Y-X order, because they result in unique Euler angles, except when $\boldsymbol{e}'_z \parallel \boldsymbol{e}_z$, e. g. for rotations about the z-axis. Then, the Euler angles are only unique up to the sum or difference of two angles.

  Fun fact: This effect is known as gimbal lock and well known in 3D graphics, where it leads to funny animation artifacts. It can be prevented by adding a 4th rotation axis or by switching to quaternion methods as explained in these Youtube videos: click, click, click.

Notes

Because of the various ambiguities wrt. rotation matrices, we agree on the following conventions:

Alibi (active) transformation
We rotate points/vectors, not the coordinate system (alias/passive transformation).

Pre-multiplication of column vectors
We use the operator form, i.e. $R\boldsymbol{x}$, where a column vector is Pre-multiplied by the matrix in contrast to post-multiplication, where a row vector is multiplied with a matrix, i.e. $\boldsymbol{x}R$.

Handedness
We use solely right-handed coordinate systems, no left-handed ones. Consequently, we may use the "right hand rule" to determine the sign of rotation angles.

Extrinsic rotations
During a composition of rotations about different angles, the coordinate system stays fixed. It is also possible to rotate it with an object, which is called intrinsic rotation.

Euler angles
For decomposing an arbitrary rotation matrix, you may use the following reference matrix (z-x-z convention)[1, §19.4], [2-4]

$$R_{z-x-z} = R_z(\gamma)R_x(\beta)R_z(\alpha) = \begin{pmatrix} c_1c_3 - s_1c_2s_3 & -s_1c_3 - c_1c_2s_3 & s_2s_3 \\ c_1s_3 + s_1c_2c_3 & -s_1s_3 + c_1c_2c_3 & -s_2c_3 \\ s_1s_2 & c_1s_2 & c_2 \end{pmatrix}, \tag{79}$$

where $s_{1/2/3}$ and $c_{1/2/3}$ are shortcuts for sine and cosine of the Euler angles α, β, γ (not Tait-Bryan angles!). Further, we agree on the ranges $\alpha \in [0, 2\pi), \beta \in [0, \pi]$ and $\gamma \in [0, 2\pi)$ in order to find unique sets (at least in case $x'_3 \neq x_3$). For a decomposition in rotations about the three Cartesian axes, you may use

$$R_{z-y-x} = R_z(\gamma)R_y(\beta)R_x(\alpha) = \begin{pmatrix} c_2c_3 & s_1s_2c_3 - c_1s_3 & c_1s_2c_3 + s_1s_3 \\ c_2s_3 & s_1s_2s_3 + c_1c_3 & c_1s_2s_3 - s_1c_3 \\ -s_2 & s_1c_2 & c_1c_2 \end{pmatrix}. \tag{80}$$

References

[1] Tilo Arens, ed. *Mathematik*. 2., korrigierter Nachdr. OCLC: 633452574. Heidelberg: Spektrum, Akad. Verl, 2010. ISBN: 978-3-8274-1758-9.

See also the following Wikipedia entries and included graphics / animations

[2] https://en.wikipedia.org/wiki/Rotation_matrix#Ambiguities

[3] https://en.wikipedia.org/wiki/Rotation_formalisms_in_three_dimensions

[4] https://en.wikipedia.org/wiki/Euler_angles

These two handouts give a good overview of the topic wrt. linear algebra

[5] robotics.caltech.edu/~jwb/courses/ME115/handouts/rotation.pdf

[6] http://scipp.ucsc.edu/~haber/ph216/rotation_12.pdf