An arbitrary rotation without matrices

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NOTE: This paper uses the nomenclature that $\boldsymbol{w}$ *is a vector and* $\hat{\boldsymbol{w}}$ *is a unit vector.*

A right-handed (RH) rotation, by some angle ψ about some axis $\hat{\boldsymbol{x}}$, can be defined without matrices. The victim vector $\boldsymbol{w}$ is projected into three pieces: ($\boldsymbol{w}_\parallel$) the piece parallel to the axis, ($\boldsymbol{w}_\perp$) the piece perpendicular to the axis, and ($\boldsymbol{w}'_\perp$), the perpendicular $\boldsymbol{w}_\perp$ rotated by 90°. The parallel piece is unaltered by the rotation, and the two $\boldsymbol{w}_\perp$ form a basis for the rotation;

$$\boldsymbol{w}' = R(\boldsymbol{w}) = \underbrace{(\boldsymbol{w}\cdot\hat{\boldsymbol{x}})\hat{\boldsymbol{x}}}_{\boldsymbol{w}_\parallel} + \cos\psi\underbrace{(\boldsymbol{w}-\boldsymbol{w}_\parallel)}_{\boldsymbol{w}_\perp} + \sin\psi\underbrace{(\hat{\boldsymbol{x}}\times\boldsymbol{w})}_{\boldsymbol{w}'_\perp}\,. \tag{1}$$

We can validate this scheme by showing it preserves the defining properties of rotations. First, the angle to the axis is unaltered;

$$\begin{aligned}\boldsymbol{w}'\cdot\hat{\boldsymbol{x}} &= (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})\cancelto{1}{\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{x}}} + \cos\psi(\boldsymbol{w}\cdot\hat{\boldsymbol{x}} - (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})\cancelto{1}{\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{x}})} + \sin\psi\cancelto{0}{((\hat{\boldsymbol{x}}\times\boldsymbol{w})\cdot\hat{\boldsymbol{x}})} \\ &= \boldsymbol{w}\cdot\hat{\boldsymbol{x}} \end{aligned} \tag{2}$$

(which uses $\boldsymbol{a}\cdot(\boldsymbol{b}\times\boldsymbol{c}) = \boldsymbol{b}\cdot(\boldsymbol{c}\times\boldsymbol{a}) = \boldsymbol{c}\cdot(\boldsymbol{a}\times\boldsymbol{b})$). Second, the vector's length is unaltered;

$$\begin{aligned}|\boldsymbol{w}'|^2 &= (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2\cancelto{1}{\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{x}}} + \cos^2\psi\,(|\boldsymbol{w}|^2 - 2(\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2 + (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2) + \sin^2\psi\,|\boldsymbol{w}|^2(|\boldsymbol{w}|^2 - (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2) \\ &= (\boldsymbol{w}\cdot\hat{\boldsymbol{x}}) + (\sin^2\psi + \cos^2\psi)(|\boldsymbol{w}|^2 - (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2) \\ &= |\boldsymbol{w}|^2 \end{aligned} \tag{3}$$

Here, we have used the identity $|\boldsymbol{u}\times\boldsymbol{v}|^2 = |\boldsymbol{u}|^2|\boldsymbol{v}|^2 - (\boldsymbol{u}\cdot\boldsymbol{v})^2$ (from $\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$), and implicitly used the orthogonality of the each component vector

$$\boldsymbol{w}_\parallel\cdot\boldsymbol{w}_\perp = (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2 - (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})^2 = 0\,, \tag{4}$$

$$\boldsymbol{w}_\perp\cdot\boldsymbol{w}'_\perp = \cancelto{0}{\boldsymbol{w}\cdot(\hat{\boldsymbol{x}}\times\boldsymbol{w})} - (\boldsymbol{w}\cdot\hat{\boldsymbol{x}})\,\cancelto{0}{\hat{\boldsymbol{x}}\cdot(\hat{\boldsymbol{x}}\times\boldsymbol{w})} = 0\,. \tag{5}$$

Instead of an axis $\hat{\boldsymbol{x}}$ and angle ψ as our input degrees of freedom, we may want the rotation that takes vector $\boldsymbol{u}\to\boldsymbol{v}$. We can reuse Eq. 1, and define:

$$\cos\psi = \hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}} \tag{6}$$

$$\sin\psi = |\boldsymbol{u}\times\boldsymbol{v}| \tag{7}$$

$$\hat{\boldsymbol{x}}_1 = \frac{\hat{\boldsymbol{u}}\times\hat{\boldsymbol{v}}}{|\hat{\boldsymbol{u}}\times\hat{\boldsymbol{v}}|} = \frac{\hat{\boldsymbol{u}}\times\hat{\boldsymbol{v}}}{\sin\psi} \tag{8}$$

However, $\hat{\boldsymbol{x}}_1$ is only one *possible* rotation axis which takes $\boldsymbol{u}\to\boldsymbol{v}$. Consider a rotation of $\psi=\pi$ about the axis bisecting the two normalized vectors

$$\hat{\boldsymbol{x}}_2 = \frac{\hat{\boldsymbol{u}}+\hat{\boldsymbol{v}}}{|\hat{\boldsymbol{u}}+\hat{\boldsymbol{v}}|} = \frac{\hat{\boldsymbol{u}}+\hat{\boldsymbol{v}}}{\sqrt{2(1+\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}})}}\,. \tag{9}$$

This rotation also clearly takes $\boldsymbol{u} \to \boldsymbol{v}$. In fact, any axis which satisfies

$$\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{x}} = \hat{\boldsymbol{v}} \cdot \hat{\boldsymbol{x}} \tag{10}$$

defines a valid rotation (since $\boldsymbol{u}$ and $\boldsymbol{v}$ will have the same latitude relative to $\hat{\boldsymbol{x}}$, and thus trace out the same circle during the rotation). Thus, "the rotation which takes $\boldsymbol{u} \to \boldsymbol{v}$" is ambiguous.

This ambiguity stems from a hidden degree of freedom. We are free to choose $(x,\, y,\, z)$ vectors

$$\boldsymbol{u} = (0,\, 0,\, 1) \tag{11}$$

$$\boldsymbol{v} = (\cos\phi\sin\theta,\, \sin\phi\sin\theta,\, \cos\theta) \tag{12}$$

We can get from $\boldsymbol{u}$ to $\boldsymbol{v}$ in two steps: (i) A RH rotation about $\hat{\boldsymbol{z}}$ by angle ϕ. (ii) A RH rotation about $\hat{\boldsymbol{y}}'$ (the new y-axis, after the first rotation) by angle θ. This procedure uses only two of the three Euler angles required to cover SO(3), the group of 3-dimensional rotations. To complete the coverage, we need a final RH rotation about $\hat{\boldsymbol{z}}''$ (the final z-axis, which in our case is the newly minted $\boldsymbol{v}$).

By construction, this post-rotation about $\boldsymbol{v}$ by angle ω cannot alter $\boldsymbol{v}$, so it does not spoil the original purpose of this rotation (take $\boldsymbol{u} \to \boldsymbol{v}$). Instead, ω determines what happens to *every other* vector, and does so by selecting *one* axis $\hat{\boldsymbol{x}}$ from the set which map $\boldsymbol{u} \to \boldsymbol{v}$. If we can find this $\hat{\boldsymbol{x}}$, we can describe the complete operation as a single rotation (instead of two sequential rotations). We have already found two valid $\hat{\boldsymbol{x}}$ (Eqs. 8 and 9), and they are fortuitously orthogonal, so we can use them to construct a basis that parameterizes all possible axes of rotation

$$\hat{\boldsymbol{x}} = a\,\hat{\boldsymbol{x}}_1 + b\,\hat{\boldsymbol{x}}_2 \tag{13}$$

Our task is now clear; given $\boldsymbol{u}$, $\boldsymbol{v}$ and ω, determine a and b to find $\hat{\boldsymbol{x}}$.

R_1 is the rotation about $\hat{\boldsymbol{x}}_1$ by $\theta = \arccos(\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}})$ and R_2 is the rotation about $\hat{\boldsymbol{x}}_2$ by ω. Applying them consecutively produces a composite rotation which cannot alter the axis of rotation;

$$\hat{\boldsymbol{x}} = R_2(R_1(\hat{\boldsymbol{x}}))\,. \tag{14}$$

Since this defining property applies to both of $\hat{\boldsymbol{x}}$'s component individually (and linearly), we can solve for a and b by using unitarity as one equation (i.e. $a^2 + b^2 = 1$), then obtain the other equation by calculating

$$\begin{aligned} a &= R_2(R_1(a\,\hat{\boldsymbol{x}}_1 + b\,\hat{\boldsymbol{x}}_2)) \cdot \hat{\boldsymbol{x}}_1 \\ &= a\,R_2(R_1(\hat{\boldsymbol{x}}_1)) \cdot \hat{\boldsymbol{x}}_1 + b\,R_2(R_1(\hat{\boldsymbol{x}}_2)) \cdot \hat{\boldsymbol{x}}_1\,. \end{aligned} \tag{15}$$

Beginning with $\hat{\boldsymbol{x}}_1$, we are lucky that R_1 does not alter it's own axis, while R_2 creates only one term parallel to $\hat{\boldsymbol{x}}_1$;

$$R_1(\hat{\boldsymbol{x}}_1) = \hat{\boldsymbol{x}}_1\ ; \tag{16}$$

$$R_2(R_1(\hat{\boldsymbol{x}}_1)) \cdot \hat{\boldsymbol{x}}_1 = \left(\left(\cancelto{0}{\hat{\boldsymbol{x}}_1 \cdot \hat{\boldsymbol{v}}}\right)\hat{\boldsymbol{v}} + \cos\omega(\hat{\boldsymbol{x}}_1 - 0) + \sin\omega\underbrace{(\hat{\boldsymbol{v}} \times \hat{\boldsymbol{x}}_1)}_{\perp \text{ to } \hat{\boldsymbol{x}}_1}\right) \cdot \hat{\boldsymbol{x}}_1 = \cos\omega \tag{17}$$

The effect on $\hat{\boldsymbol{x}}_2$ is slightly more complicated;

$$\begin{aligned} R_1(\hat{\boldsymbol{x}}_2) &= \left(\left(\cancelto{0}{\hat{\boldsymbol{x}}_2 \cdot \hat{\boldsymbol{x}}_1}\right)\hat{\boldsymbol{x}}_1 + \cos\theta(\hat{\boldsymbol{x}}_2 - 0) + \sin\theta(\hat{\boldsymbol{x}}_1 \times \hat{\boldsymbol{x}}_2)\right. \\ &= \frac{1}{\sqrt{2(1+\cos(\theta))}}\left(\cos\theta\,(\hat{\boldsymbol{u}} + \hat{\boldsymbol{v}}) + \sin\theta\,\frac{(\hat{\boldsymbol{u}} \times \hat{\boldsymbol{v}})}{\sin\theta} \times (\hat{\boldsymbol{u}} + \hat{\boldsymbol{v}})\right) \\ &= \frac{1}{\sqrt{2(1+\cos(\theta))}}\left(\cos\theta\,(\hat{\boldsymbol{u}} + \hat{\boldsymbol{v}}) + \hat{\boldsymbol{v}} - \hat{\boldsymbol{u}}\cos\theta + \hat{\boldsymbol{v}}\cos\theta - \hat{\boldsymbol{u}}\right) \\ &= \frac{1}{\sqrt{2(1+\cos(\theta))}}\left((2\cos\theta + 1)\hat{\boldsymbol{v}} - \hat{\boldsymbol{u}}\right) \end{aligned} \tag{18}$$

(using $(\boldsymbol{a} \times \boldsymbol{b}) \times \boldsymbol{c} = \boldsymbol{b}(\boldsymbol{a} \cdot \boldsymbol{c}) - \boldsymbol{a}(\boldsymbol{b} \cdot \boldsymbol{c})$). Before we put all of Eq. 18 through R_2, we should recall that the final equation only uses terms parallel to $\hat{\boldsymbol{x}}_1$. R_2 only returns terms which are (i) parallel to the incoming vector (which in this case is in the uv-plane, and thus orthogonal to $\hat{\boldsymbol{x}}_1$), (ii) parallel to $\hat{\boldsymbol{v}}$ (also in the uv plane) and (iii) perpendicular to $\hat{\boldsymbol{v}}$ (via $\hat{\boldsymbol{v}} \times \boldsymbol{w}$). Hence, only the 3$^{\text{rd}}$ piece is meaningful, and since $\hat{\boldsymbol{v}} \times \hat{\boldsymbol{v}} = 0$, we only need to give it Eq. 18's $\hat{\boldsymbol{u}}$ term;

$$\begin{aligned} R_2(R_1(\hat{\boldsymbol{x}}_2)) \cdot \hat{\boldsymbol{x}}_1 &= \frac{1}{\sqrt{2(1+\cos(\theta))}} R_2(-\hat{\boldsymbol{u}}) \cdot \hat{\boldsymbol{x}}_1 = \frac{1}{\sqrt{2(1+\cos(\theta))}} (\hat{\boldsymbol{v}} \times (-\hat{\boldsymbol{u}})) \cdot \hat{\boldsymbol{x}}_1 \\ &= \sin\omega \frac{\sin\theta}{\sqrt{2(1+\cos(\theta))}} \end{aligned} \tag{19}$$

(using $\hat{\boldsymbol{u}} \times \hat{\boldsymbol{v}} = \sin\theta\, \hat{\boldsymbol{x}}_1$). Combining Eq. 15, 16 and 19 we get

$$a = a\cos\omega + b\sin\omega \frac{\sin\theta}{\sqrt{2(1+\cos(\theta))}} \tag{20}$$

Having done the hard work, we can plug our system of equations into Mathematica to obtain

$$a = 2\cos(\omega/2) \frac{\sin(\theta/2)}{c(\theta)} \tag{21}$$

$$b = 2\sin(\omega/2) \frac{1}{c(\theta)} \tag{22}$$

$$c(\theta) = \sqrt{3 - \cos(\omega) - \cos(\theta)(1+\cos(\omega))} \tag{23}$$

I then used Mathematica to validate this solution by checking that $\hat{\boldsymbol{x}}$ matches the eigenvector of the composite rotation $R_2(R_1(\boldsymbol{w}))$. However, $c(\theta)$ is numerically unstable if used naïvely, due to the cosine cancellations. These terms should be rewritten in a form which *doubles* the precision of the floating point result

$$1 - \cos(t) \mapsto 2\sin^2(t/2)\,. \tag{24}$$

This gives us

$$c(\theta) \mapsto \sqrt{2\sin^2(\theta/2) + 2\sin^2(\omega/2) + (1 - \cos(\theta)\cos(\omega))}\,. \tag{25}$$

The final cancellation can be corrected using

$$\cos(\theta)\cos(\omega) = \frac{1}{2}(\cos(\theta+\omega) + \cos(\theta-\omega))\,; \tag{26}$$

$$(1 - \cos(\theta)\cos(\omega)) \mapsto \frac{1}{2}(1 - \cos(\theta+\omega)) + \frac{1}{2}(1 - \cos(\theta-\omega))\,. \tag{27}$$

Again using Eq. 24, we obtain the final expression

$$c(\theta) \mapsto \sqrt{2\sin^2(\theta/2) + 2\sin^2(\omega/2) + \sin^2(\theta+\omega) + \sin^2(\theta-\omega)}\,. \tag{28}$$

Given $\boldsymbol{u}$, $\boldsymbol{v}$ and ω, we now have the tools to find the axis $\hat{\boldsymbol{x}}$ about which the composite rotations occur.[1] But what is the angle ψ of rotation? We can determine ψ empirically by projecting $\hat{\boldsymbol{u}}$ and $\hat{\boldsymbol{v}}$ into the plane of rotation (e.g. $\hat{\boldsymbol{u}}_\perp = \hat{\boldsymbol{u}} - (\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{x}})\hat{\boldsymbol{x}}$). The rotation angle is then defined via

$$\psi = \operatorname{atan2}(\sin\psi, \cos\psi) = \operatorname{atan2}\left(\operatorname{sign}(a)|\hat{\boldsymbol{u}}_\perp \times \hat{\boldsymbol{v}}_\perp|,\ \hat{\boldsymbol{u}}_\perp \cdot \hat{\boldsymbol{v}}_\perp\right)\,. \tag{29}$$

[1] There is one class of system where $\hat{\boldsymbol{x}}$ remains ambiguous; when $\boldsymbol{u}$ and $\boldsymbol{v}$ are antiparallel, $\hat{\boldsymbol{x}}_1$ and $\hat{\boldsymbol{x}}_2$ are both null. If $\boldsymbol{x}$ is supplied externally, ω rotates it around the shared uv axis, but $\boldsymbol{x}$ cannot be determined from ω alone.

It is best to use atan2 because it is more precise for angles near 0, $\pi/2$ and π. Note that we have to inject the *sign* of a into $\sin(\psi)$, because when $a < 0$, the RH rotation becomes larger than π, so we must instead uses a *negative* RH rotation.

I have tested an implementation of this algorithm and it works quite well (it is both length and angle preserving). I have additionally validated that rotating once about $\hat{\boldsymbol{x}}$ gives the same result as the two-step composite rotation.