Derivation of the Proper Rotation $R$ that minimizes FRE

We have already shown the importance of singular value decomposition of the cross-covariance matrix, $XY^T = UV^T$, where $V^TV = I$, $U^TU = I$, $\Lambda = \text{diag}(\Lambda_1, \Lambda_2, \Lambda_3)$, and $\Lambda_1 \geq \Lambda_2 \geq \Lambda_3 \geq 0$. With it, we were able to show that FRE is minimized when $\text{tr}(V'RUA)$ is maximized, subject to $R'R = I$.

Now, we let $D \equiv \text{diag}(1,1,\det(VU))$, and note that $D'D = I$. Then, maximizing $\text{tr}(V'RUA)$ is equivalent to maximizing $\text{tr}(V'RUD'D\Lambda)$.

We define $Z \equiv V'RUD'$, so that maximizing $\text{tr}(V'RUD'D\Lambda)$ is equivalent to maximizing $\text{tr}(ZDA)$. We note that $Z'Z = I$ and that
\[
\det(Z) = \det(V'RUD') = \det(R)\det(VU)\det(D) = \det(R)\det(VU) = \det(R).
\]

Therefore, if we force $Z$ to be proper, then $R$ will also be proper. We can force $Z$ to be proper by requiring $Z$ to have the form of Eq. (8.3) of FHM:
\[
Z = \begin{bmatrix}
   \omega_x^2v + c & \omega_x\omega_y v - \omega_zs & \omega_x\omega_z v + \omega_ys \\
   \omega_x\omega_y v + \omega_zs & \omega_y^2v + c & \omega_y\omega_z v - \omega_xs \\
   \omega_x\omega_z v - \omega_ys & \omega_y\omega_z v + \omega_xs & \omega_z^2v + c
\end{bmatrix},
\]
where $c \equiv \cos(\theta), v \equiv 1 - c, s \equiv \sin(\theta)$. Using Eq. (2) gives
\[
\text{tr}(ZDA) = v(\omega_x^2\Lambda_1 + \omega_y^2\Lambda_2 + \det(UV)\omega_z^2\Lambda_3) + c(\Lambda_1 + \Lambda_2 + \det(UV)\Lambda_3).
\]

We note that $v \geq 0$, $\omega_x^2 + \omega_y^2 + \omega_z^2 = 1$, $\Lambda_1 \geq \Lambda_2 \geq \Lambda_3 \geq 0$, and $|\det(UV)| = 1$. Therefore, the first term is maximized by setting $\omega_x = 1, \omega_y = \omega_z = 0$. Inserting these values and noting that $v + c = 1$, we get
\[
\text{tr}(ZDA) = \Lambda_1 + c(\Lambda_2 + \det(UV)\Lambda_3).
\]

Finally, since $\Lambda_2 \geq \Lambda_3$ and $|\det(UV)| = 1$, we know that $(\Lambda_2 + \det(UV)\Lambda_3) \geq 0$. Therefore, to maximize $\text{tr}(ZDA)$, we must set $c = 1$, which means $\cos(\theta) = 1$, which means that $s$, which equals $\sin(\theta)$ in Eq. (2), is equal to zero. Using $c = 1, s = 0, \omega_x = 1, \omega_y = \omega_z = 0$ in Eq. (2), yields $Z = I$, and therefore,
\[
R = VDU' = V\text{diag}(1,1,\det(UV))U'.
\]