SINGULARITY-FREE COMPUTATION OF QUATERNIONS FROM ROTATION MATRICES IN $\mathbb{E}^4$ AND $\mathbb{E}^3$

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ABSTRACT. A real orthogonal matrix representing a rotation in $\mathbb{E}^4$ can be decomposed into the commutative product of a left-isoclinic and a right-isoclinic rotation matrix. The double quaternion representation of rotations in $\mathbb{E}^4$ follows directly from this decomposition. In this paper, it is shown how this decomposition can be performed without divisions. This avoids the common numerical issues attributed to the computation of quaternions from rotation matrices.

The map from the 4×4 rotation matrices to the set of double unit quaternions is a 2-to-1 covering map. Thus, this map cannot be smoothly inverted. As a consequence, it is erroneously assumed that all inversions should necessarily contain singularities that arise in the form of quotients where the divisor can be arbitrarily small. This misconception is herein clarified.

When particularized to three dimensions, it is shown how the resulting formulation outperforms, from the numerical point of view, the celebrated Shepperd's method.

1. INTRODUCTION

Any rotation in $\mathbb{E}^4$ can be seen as the composition of two rotations in a pair of orthogonal two-dimensional subspaces [1]. When the module of the rotated angles in these two subspaces are equal, the rotation is said to be *isoclinic*. It can be proved that any rotation in $\mathbb{E}^4$ can be factored into the commutative composition of two isoclinic rotations. Cayley realized this fact when studying the double quaternion representation of rotations in $\mathbb{E}^4$ [2]. The development of the first effective procedure for computing this factorization is attributed in [3] to Van Elfrinkhof [4]. Since this work, written in Dutch, remained unnoticed, other sources (see, for example, [5]) attribute it to Rosen [6]. The methods of Elfrinkhof and Rosen are equivalent (see [3, 7] for a detailed explanation). Although formally correct, these methods were not designed taking into account numerical issues. In this paper, we introduce a slight variation on them which leads to division-free closed formulas for the elements of the double quaternion corresponding to a rotation matrix in $\mathbb{E}^4$. This has interesting consequences when particularized to rotations in $\mathbb{E}^3$. We show how the resulting formulation outperforms, from the numerical point of view, the celebrated Shepperd's method widely used in aerial navigation, computer graphics, and robotics.

This paper is organized as follows. Section 2 summarizes the basic facts about rotations in $\mathbb{E}^4$ that are used in Section 3 to derive a set of division-free formulas for obtaining the double quaternion representation of a rotation in $\mathbb{E}^4$. Then, in Section 4, this result is particularized

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to rotations in $\mathbb{E}^3$. Section 5 briefly reviews Shepperd's method, the standard method used to compute the quaternion corresponding to a 3×3 rotation matrix. Section 6 compares the new method and Shepperd's method from the numerical point of view using a statistical analysis. Section 7 summarizes the main points.

2. Rotations in $\mathbb{E}^4$

The elements of the Lie group of rotations in four-dimensional space, $SO(4)$, can be either simple or double rotations. Simple rotations have an invariant plane of points, while double rotations have a single invariant point only, the center of rotation. In addition, double rotations present at least a couple of invariant planes that are orthogonal. Then, a rotation in $\mathbb{E}^4$ has two angles of rotation, α_1 and α_2, one for each plane of rotation, through which points in the planes rotate. All points not in the planes rotate through an angle between α_1 and α_2. See [8] for details on the geometric interpretation of rotations in four dimensions.

Isoclinic rotations are a particular case of double rotations in which there are infinitely many invariant orthogonal planes, with same rotation angles, that is, $\alpha_1 = \pm\alpha_2$. These rotations can be left-isoclinic, when the rotation in both planes is the same ($\alpha_1 = \alpha_2$), or right-isoclinic, when the rotations in both planes have opposite signs ($\alpha_1 = -\alpha_2$).

Isoclinic rotation have several important properties: (a) the composition of two right- (left-) isoclinic rotations is a right- (left-) isoclinic rotation; (b) the composition of a right- and a left-isoclinic rotation is commutative; and (c) any 4D rotation can be decomposed into the composition of a right- and a left-isoclinic rotations.

Right- and a left-isoclinic rotations form maximal and normal subgroups. Denote S^3_R as the subgroups of right-isoclinic rotations, and S^3_R the subgroup of left-isoclinic rotations. The direct product $S^3_L \times S^3_R$ is a double cover of the group $SO(4)$, as four-dimensional rotations can be seen as the composition of rotations of these two subgroups, and there are two expressions for each element of the group.

The left- and right-isoclinic rotations can be represented by rotation matrices of the form

$$\mathbf{R}^L = \begin{pmatrix} l_0 & -l_3 & l_2 & -l_1 \\ l_3 & l_0 & -l_1 & -l_2 \\ -l_2 & l_1 & l_0 & -l_3 \\ l_1 & l_2 & l_3 & l_0 \end{pmatrix}, \tag{1}$$

and

$$\mathbf{R}^R = \begin{pmatrix} r_0 & -r_3 & r_2 & r_1 \\ r_3 & r_0 & -r_1 & r_2 \\ -r_2 & r_1 & r_0 & r_3 \\ -r_1 & -r_2 & -r_3 & r_0 \end{pmatrix}, \tag{2}$$

respectively, where

$$\mathbf{l} = \sigma(l_0, l_1, l_2, l_3), \tag{3}$$

$$\mathbf{r} = \sigma(r_0, r_1, r_2, r_3), \tag{4}$$

directly correspond to their quaternion representation with $\sigma = \pm 1$.

Since (1) and (2) are rotation matrices, their rows and columns are unit vectors. As a consequence,

$$l_0^2 + l_1^2 + l_2^2 + l_3^2 = 1, \tag{5}$$

$$r_0^2 + r_1^2 + r_2^2 + r_3^2 = 1. \tag{6}$$

and the quaternions in (3) and (4) are unit quaternions.

Without loss of generality, we have introduced some changes in the signs and indices of (1) and (2) with respect to the notation used by Cayley [2, 5] to provide a neat connection with the standard use of quaternions for representing rotations in three dimensions.

According to the above properties, a 4D rotation matrix, say $\mathbf{R}$, can be expressed as:

$$\mathbf{R} = \mathbf{R}^L\mathbf{R}^R = \mathbf{R}^R\mathbf{R}^L, \tag{7}$$

where

$$\mathbf{R}^L = l_0\mathbf{I} + l_1\mathbf{A}_1 + l_2\mathbf{A}_2 + l_3\mathbf{A}_3, \tag{8}$$

and

$$\mathbf{R}^R = r_0\mathbf{I} + r_1\mathbf{B}_1 + r_2\mathbf{B}_2 + r_3\mathbf{B}_3, \tag{9}$$

where $\mathbf{I}$ stands for the 4×4 identity matrix and

$$\mathbf{A}_1 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{A}_3 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\mathbf{B}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{B}_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \mathbf{B}_3 = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

Now, it can be verified that

$$\mathbf{A}_1^2 = \mathbf{A}_2^2 = \mathbf{A}_3^2 = \mathbf{A}_1\mathbf{A}_2\mathbf{A}_3 = -\mathbf{I}, \tag{10}$$

and

$$\mathbf{B}_1^2 = \mathbf{B}_2^2 = \mathbf{B}_3^2 = \mathbf{B}_1\mathbf{B}_2\mathbf{B}_3 = -\mathbf{I}. \tag{11}$$

Expression (10) determines all the possible products of $\mathbf{A}_1$, $\mathbf{A}_2$, and $\mathbf{A}_3$ resulting in

$$\begin{aligned} &\mathbf{A}_1\mathbf{A}_2 = \mathbf{A}_3, \quad &\mathbf{A}_2\mathbf{A}_3 = \mathbf{A}_1, \quad &\mathbf{A}_3\mathbf{A}_1 = \mathbf{A}_2, \\ &\mathbf{A}_2\mathbf{A}_1 = -\mathbf{A}_3, \quad &\mathbf{A}_3\mathbf{A}_2 = -\mathbf{A}_1, \quad &\mathbf{A}_1\mathbf{A}_3 = -\mathbf{A}_2. \end{aligned} \tag{12}$$

Likewise, all the possible products of $\mathbf{B}_1$, $\mathbf{B}_2$, and $\mathbf{B}_3$ can be derived from expression (11). Moreover, it can be verified that

$$\mathbf{A}_i\mathbf{B}_j = \mathbf{B}_j\mathbf{A}_i. \tag{13}$$

which is actually a consequence of the commutativity of left- and right-isoclinic rotations.

3. The proposed factorization method

The problem of factoring a 4D rotation matrix, say $\mathbf{R}$, into the product of a right- and a left-isoclinic rotation matrix consists in finding the values of $l_0,\ldots,l_3$ and $r_0,\ldots,r_3$ that satisfy the following matrix equation:

$$\mathbf{R} = \begin{pmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ r_{21} & r_{22} & r_{23} & r_{24} \\ r_{31} & r_{32} & r_{33} & r_{34} \\ r_{41} & r_{42} & r_{43} & r_{44} \end{pmatrix} = \begin{pmatrix} l_0 & -l_3 & l_2 & -l_1 \\ l_3 & l_0 & -l_1 & -l_2 \\ -l_2 & l_1 & l_0 & -l_3 \\ l_1 & l_2 & l_3 & l_0 \end{pmatrix} \begin{pmatrix} r_0 & -r_3 & r_2 & r_1 \\ r_3 & r_0 & -r_1 & r_2 \\ -r_2 & r_1 & r_0 & r_3 \\ -r_1 & -r_2 & -r_3 & r_0 \end{pmatrix}. \tag{14}$$

To this end, let us first define the *matrix of products* as:

$$\mathbf{P}_4 := \begin{pmatrix} l_0 \\ l_1 \\ l_2 \\ l_3 \end{pmatrix} \begin{pmatrix} r_0 & r_1 & r_2 & r_3 \end{pmatrix} = \begin{pmatrix} l_0r_0 & l_0r_1 & l_0r_2 & l_0r_3 \\ l_1r_0 & l_1r_1 & l_1r_2 & l_1r_3 \\ l_2r_0 & l_2r_1 & l_2r_2 & l_2r_3 \\ l_3r_0 & l_3r_1 & l_3r_2 & l_3r_3 \end{pmatrix}. \tag{15}$$

Observe that the norm of row i of this matrix is:

$$+\sqrt{l_{i+1}^2(r_0^2+r_1^2+r_2^2+r_3^2)} = |l_{i+1}|. \tag{16}$$

Likewise, the norm of column i is:

$$+\sqrt{r_{i+1}^2(l_0^2+l_1^2+l_2^2+l_3^2)} = |r_{i+1}|. \tag{17}$$

Now, using equation (14), it can be verified that[1]:

(18)

$$\mathbf{P}_4 = \frac{1}{4}\begin{pmatrix} r_{11}+r_{22}+r_{33}+r_{44} & -r_{41}+r_{32}-r_{23}+r_{14} & -r_{31}-r_{42}+r_{13}+r_{24} & r_{21}-r_{12}-r_{43}+r_{34} \\ r_{41}+r_{32}-r_{23}-r_{14} & r_{11}-r_{22}-r_{33}+r_{44} & r_{21}+r_{12}+r_{43}+r_{34} & r_{31}-r_{42}+r_{13}-r_{24} \\ -r_{31}+r_{42}+r_{13}-r_{24} & r_{21}+r_{12}-r_{43}-r_{34} & -r_{11}+r_{22}-r_{33}+r_{44} & r_{41}+r_{32}+r_{23}+r_{14} \\ r_{21}-r_{12}+r_{43}-r_{34} & r_{31}+r_{42}+r_{13}+r_{24} & -r_{41}+r_{32}+r_{23}-r_{14} & -r_{11}-r_{22}+r_{33}+r_{44} \end{pmatrix}.$$

Therefore, the norms of the row and column vectors of the matrix in (18) gives us the modules of $l_0,\dots,l_3$ and $r_0,\dots,r_3$. To assign a consistent set of signs to them, we can take any positive entry in the matrix given in (18), say $p_{k,l}$. Then, according to (15), l_{k-1} and r_{l-1} are both positive or negative. If we assume that they are both positive, then we have that:

$$\text{sign}(l_{i-1}) = \text{sign}(p_{i,l}), i \in \{1,2,3,4\}\backslash k, \tag{19}$$

and

$$\text{sign}(r_{j-1}) = \text{sign}(p_{k,j}), j \in \{1,2,3,4\}\backslash l. \tag{20}$$

Another set of consistent signs are obtained if we assume that l_{k-1} and r_{l-1} are both negative, thus accounting for the double covering of the space of rotations.

4. Particularization to $\mathbb{E}^3$

A 4×4 rotation matrix, when representing a rotation in a 3-dimensional subspace, can be expressed as:

$$\mathbf{R} = \begin{pmatrix} r_{11} & r_{12} & r_{13} & 0 \\ r_{21} & r_{22} & r_{23} & 0 \\ r_{31} & r_{32} & r_{33} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

Therefore, in this case, (18) reduces to:

$$\mathbf{P}_3 = \frac{1}{4}\begin{pmatrix} r_{11}+r_{22}+r_{33}+1 & r_{32}-r_{23} & r_{13}-r_{31} & r_{21}-r_{12} \\ r_{32}-r_{23} & r_{11}-r_{22}-r_{33}+1 & r_{21}+r_{12} & r_{31}+r_{13} \\ r_{13}-r_{31} & r_{21}+r_{12} & r_{22}-r_{11}-r_{33}+1 & r_{32}+r_{23} \\ r_{21}-r_{12} & r_{31}+r_{13} & r_{32}+r_{23} & r_{33}-r_{11}-r_{22}+1 \end{pmatrix}. \tag{22}$$

Due to the symmetry of this matrix, $l_i = r_i$, $i = 0,\dots,3$. As we already knew, the double quaternion representation of rotations in $\mathbb{E}^4$ reduces to a single quaternion representation in $\mathbb{E}^3$.

[1]The expression given in [7] for this matrix is incorrect.

Let us denote this quaternion by $\mathbf{q} = (q_0, q_1, q_2, q_3)$. Therefore, computing the norms of the rows or the columns of (22), we have that:

$$|q_0| = +\frac{1}{4}\sqrt{(r_{11}+r_{22}+r_{33}+1)^2+(r_{32}-r_{23})^2+(r_{13}-r_{31})^2+(r_{21}-r_{12})^2}, \tag{23}$$

$$|q_1| = +\frac{1}{4}\sqrt{(r_{32}-r_{23})^2+(r_{11}-r_{22}-r_{33}+1)^2+(r_{21}+r_{12})^2+(r_{31}+r_{13})^2}, \tag{24}$$

$$|q_2| = +\frac{1}{4}\sqrt{(r_{13}-r_{31})^2+(r_{21}+r_{12})^2+(r_{22}-r_{11}-r_{33}+1)^2+(r_{32}+r_{23})^2}, \tag{25}$$

$$|q_3| = +\frac{1}{4}\sqrt{(r_{21}-r_{12})^2+(r_{31}+r_{13})^2+(r_{32}+r_{23})^2+(r_{33}-r_{11}-r_{22}+1)^2}. \tag{26}$$

If we assume that q_0 is positive, we can give a consistent set of signs to the other elements of the quaternion by simply assigning the signs of $(r_{32}-r_{23})$, $(r_{13}-r_{31})$, and $(r_{21}-r_{12})$, to q_1, q_2, and q_3, respectively.

5. Shepperd's method

Since it was first proposed in [9], Shepperd's method remains as one of the most popular methods for computing the quaternion corresponding to a 3×3 rotation matrix. It improves on Hughes' method [10] via a voting scheme. In this method, there are four different formulas for computing the quaternion as a function of the entries of the rotation matrix, all of them formally equivalent. Numerically, however, these four formulas are not identical and, depending on the rotation matrix, one of them is numerically better conditioned than the others. These four formulas are:

$$\mathbf{u}_1 = \frac{1}{2}\begin{pmatrix} (1+r_{11}+r_{22}+r_{33})^{\frac{1}{2}} \\ (r_{32}-r_{23})/(1+r_{11}+r_{22}+r_{33})^{\frac{1}{2}} \\ (r_{13}-r_{31})/(1+r_{11}+r_{22}+r_{33})^{\frac{1}{2}} \\ (r_{21}-r_{12})/(1+r_{11}+r_{22}+r_{33})^{\frac{1}{2}} \end{pmatrix}, \tag{27}$$

$$\mathbf{u}_2 = \frac{1}{2}\begin{pmatrix} (r_{32}-r_{23})/(1+r_{11}-r_{22}-r_{33})^{\frac{1}{2}} \\ (1+r_{11}-r_{22}-r_{33})^{\frac{1}{2}} \\ (r_{12}+r_{21})/(1+r_{11}-r_{22}-r_{33})^{\frac{1}{2}} \\ (r_{31}+r_{13})/(1+r_{11}-r_{22}-r_{33})^{\frac{1}{2}} \end{pmatrix}, \tag{28}$$

$$\mathbf{u}_3 = \frac{1}{2}\begin{pmatrix} (r_{13}-r_{31})/(1-r_{11}+r_{22}-r_{33})^{\frac{1}{2}} \\ (r_{12}+r_{21})/(1-r_{11}+r_{22}-r_{33})^{\frac{1}{2}} \\ (1-r_{11}+r_{22}-r_{33})^{\frac{1}{2}} \\ (r_{23}+r_{32})/(1-r_{11}+r_{22}-r_{33})^{\frac{1}{2}} \end{pmatrix}, \tag{29}$$

$$\mathbf{u}_4 = \frac{1}{2}\begin{pmatrix} (r_{21}-r_{12})/(1-r_{11}-r_{22}+r_{33})^{\frac{1}{2}} \\ (r_{31}+r_{13})/(1-r_{11}-r_{22}+r_{33})^{\frac{1}{2}} \\ (r_{32}+r_{23})/(1-r_{11}-r_{22}+r_{33})^{\frac{1}{2}} \\ (1-r_{11}-r_{22}+r_{33})^{\frac{1}{2}} \end{pmatrix}. \tag{30}$$

When computing any of the above solutions, numerical issues arise when square rooting, or when dividing by, very small numbers [11]. To obtain the better conditioned solution for each case, the ordinal number i of the largest element in the following vector is determined:

$$\begin{pmatrix} r_{11}+r_{22}+r_{33} \\ r_{11} \\ r_{22} \\ r_{33} \end{pmatrix}. \tag{31}$$

Then, the best solution, from the numerical point of view, is considered to be $\mathbf{u}_i$.

6. Comparison

To compare the performance of the derived method with Shepperd's method, we perform a statistical analysis using single-precision floating-point arithmetics in MATLAB®. We generate 10^6 random unit quaternions using the algorithm described in [12] (it actually permits generating uniformly distributed points in $\mathbb{S}^4$). For each generated quaternion, we obtain the corresponding rotation matrix using Rodrigues' formula, and then we recover the original quaternion using Shepperd's and the proposed method. The error committed in both cases is evaluated as the norm of the vector difference between the original and recovered quaternions. In general, this is not a good way to compute the distance between two quaternions. Nevertheless, since in our case the error is assumed to be very small, the length of the vector connecting both orientations in $\mathbb{S}^4$ is going to coincide with the value of the angle formed by them if seen from the center of $\mathbb{S}^4$ (and this angle can be taken as a distance between any two elements of the 3D rotation group $SO(3)$ [13]).

TABLE 1. Error and time performances of Shepperd's and the new method.

Method	Quaternions recovered without error	Worst-case error $\times 10^{-7}$	Average error $\times 10^{-8}$	Standard deviation $\times 10^{-8}$	Average time (μs)	Best-case time (μs)
Shepperd's	21.7%	1.35	3.35	4.42	14.04	11.99
New method	31.9%	1.23	2.15	3.26	83.22	74.88

The time and error performances of the two described methods are compiled in Table 1. In this table, the first four columns refer to the error performance. The first one shows the percentage of cases in which the original quaternion is recovered without error. The other three correspond to the error committed in the worst-case, the average error, and the standard deviation of the error, respectively. Finally, we have two columns with the time performance. The first column gives the average time required to compute a quaternion from a rotation matrix; and the second column, the time required in the best of the cases. The worst-case time is not included because it is meaningless on a multitasking machine. These results have been obtained with a MATLAB® implementation running on an Intel® Core™i2 with 8 GB of RAM.

7. Conclusion

A singularity-free formulation for computing the double and single quaternion corresponding to a given rotation in $\mathbb{E}^4$ and $\mathbb{E}^3$, respectively, has been presented. The three-dimensional version of this formulation has been shown to numerically outperform Shepperd's method. In particular, if we take a quaternion at random and we compute the corresponding rotation matrix, the probability of recovering exactly the original quaternion from this matrix using Shepperd's method is about 22%, while using the new method this probability is increased to 32%. As a counterpart, the computational cost of the proposed method is about six times higher than that of Shepperd's, which does not seem to be a major limitation for modern computer technology.

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