The Journal of the Astronautical Sciences, Vol. 41, No. 4, October-December 1993, pp. 545–556

Quaternion Computation from a Geometric Point of View

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Abstract

Global algorithms that solve for the quaternion generally have a four-fold multiplicity in order to avoid singularities. A geometrically-motivated construction is presented that automatically generates the four-fold multiplicity of algorithms once a single (possibly singular) algorithm is known. As examples of the application of this procedure, least-squares attitude determination and the computation of the quaternion from the direction-cosine matrix are examined. In the latter application, the method proposed here leads to Shepperd's algorithm for extracting the quaternion from the rotation matrix.

Introduction

The computation of the quaternion (more correctly, Euler-Rodrigues symmetric parameters) [1],

$$\bar{\eta} = \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{bmatrix}, \tag{1}$$

in attitude problems is complicated by the fact that the four components of the quaternion are not all independent but satisfy the constraint

$$\bar{\eta}^T\bar{\eta} \equiv \eta_1^2 + \eta_2^2 + \eta_3^2 + \eta_4^2 = 1\,, \tag{2}$$

Therefore, in computations of the quaternion one must either utilize all four components, while taking the quaternion normalization constraint into account explicitly, or one must reduce the problem to one of lower dimension. The former approach is not possible in general because the operations which we perform on

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the quaternion are usually not norm-preserving. Therefore, we must almost always at some point replace the quaternion by a three-dimensional representation, usually the Rodrigues (or Gibbs) vector [1]. However, as has been shown by Stuelpnagel [2], any attitude representation of three dimensions is necessarily singular at some point. Thus, even though the quaternion is nonsingular, the algorithms which we use to calculate it are often singular.

A well-known example of this "singularity" phenomenon in the nonsingular quaternion is the computation of the quaternion from the direction-cosine matrix [3–9], for which one must solve the equation

$$A = \begin{bmatrix} \eta_1^2 - \eta_2^2 - \eta_3^2 + \eta_4^2 & 2(\eta_1\eta_2 + \eta_4\eta_3) & 2(\eta_1\eta_3 - \eta_4\eta_2) \\ 2(\eta_2\eta_1 - \eta_4\eta_3) & -\eta_1^2 + \eta_2^2 - \eta_3^2 + \eta_4^2 & 2(\eta_2\eta_3 + \eta_4\eta_1) \\ 2(\eta_3\eta_1 + \eta_4\eta_2) & 2(\eta_3\eta_2 - \eta_4\eta_1) & -\eta_1^2 - \eta_2^2 + \eta_3^2 + \eta_4^2 \end{bmatrix} . \tag{3}$$

Here, it turns out that the component of the quaternion that is calculated first is treated very differently from the remaining three (see Application 2 below). Since one can solve for any of the four components first, there are four different algorithms for computing the quaternion as a function of the direction-cosine matrix, all of them formally equivalent (within an undetermined but physically unimportant overall sign). Numerically, however, these four algorithms are not identical, and, depending on the specific value of the direction-cosine matrix, one or more of these four algorithms may entail an unacceptable loss of significance. These algorithms are studied in greater detail later in this work.

The four-fold multiplicity of algorithms also arises commonly in the development of an intermediate solution in terms of a three-dimensional representation, which we now develop in some detail. Most attitude problems begin with the study of some function of the attitude matrix A, which may be either scalar, $F(A)$, or vectorial, $\mathbf{F}(A)$. Generally, one looks for a value of the attitude matrix, A^*, that either minimizes a scalar function,

$$F(A^*) \leq F(A) \quad \forall A , \tag{4}$$

or is a "root" of a vectorial function

$$\mathbf{F}(A^*) = \mathbf{0} . \tag{5}$$

If the attitude matrix is parameterized in terms of some three-dimensional representation $\mathbf{p}$, and the value, $\mathbf{p}^*$, that corresponds to A^* does not lie on the boundary of definition of $\mathbf{p}$, then equation (4) leads to

$$\frac{\partial F}{\partial \mathbf{p}}(A(\mathbf{p})) = \mathbf{0} \quad \text{at} \quad \mathbf{p} = \mathbf{p}^*, \tag{6}$$

which is very much in the form of equation (5). Most attitude problems at some stage of their development have the form of equation (5).

Equations (4) or (5) can be transformed into equations for the quaternion by means of the substitution given by equation (3), which leads to equivalent equations for the quaternion

$$f(\bar{\eta}^*) = F(A(\bar{\eta}^*)) \le f(\bar{\eta}) \quad \forall\, \bar{\eta}, \tag{7a}$$

or

$$\mathbf{f}(\bar{\eta}^*) \equiv \mathbf{f}(\eta_1^*, \eta_2^*, \eta_3^*, \eta_4^*) = \mathbf{0}. \tag{7b}$$

Consider now the intermediate solution of equation (7b) in terms of the Rodrigues vector, defined as

$$\boldsymbol{\rho} \equiv \boldsymbol{\eta}/\eta_4 = \frac{1}{\eta_4}\begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}, \tag{8}$$

which leads to

$$\mathbf{g}(\boldsymbol{\rho}^*) \equiv \mathbf{f}\left(\frac{\rho_1^*}{\sqrt{1+|\boldsymbol{\rho}^*|^2}}, \frac{\rho_2^*}{\sqrt{1+|\boldsymbol{\rho}^*|^2}}, \frac{\rho_3^*}{\sqrt{1+|\boldsymbol{\rho}^*|^2}}, \frac{1}{\sqrt{1+|\boldsymbol{\rho}^*|^2}}\right) = \mathbf{0}. \tag{9}$$

Once the desired solution, $\boldsymbol{\rho}^*$, has been determined, the associated quaternion solution, $\bar{\eta}^*$, can be reconstructed according to

$$\bar{\eta}^* = \frac{1}{\sqrt{1+|\boldsymbol{\rho}^*|^2}}\begin{bmatrix} \boldsymbol{\rho}^* \\ 1 \end{bmatrix}. \tag{10}$$

This program works well, however, only when η_4^* is significantly different from zero. Otherwise, even if η_4^* is nonvanishing, $|\boldsymbol{\rho}^*|$ must be very large when η_4^* is close to zero, indicating that the equations for $\boldsymbol{\rho}^*$ must be nearly singular. The solution for $\boldsymbol{\rho}^*$ and, therefore, $\bar{\eta}^*$ must suffer from a substantial loss of numerical significance. The remedy in this case is to divide out a different component, say η_1, and define a vector, $\boldsymbol{\alpha} \equiv [\alpha_2, \alpha_3, \alpha_4]^T$, according to

$$\alpha_2 = \eta_2/\eta_1, \quad \alpha_3 = \eta_3/\eta_1 \quad \text{and} \quad \alpha_4 = \eta_4/\eta_1, \tag{11}$$

which leads to

$$\mathbf{g}'(\boldsymbol{\alpha}^*) \equiv \mathbf{f}\left(\frac{1}{\sqrt{1+|\boldsymbol{\alpha}^*|^2}}, \frac{\alpha_2^*}{\sqrt{1+|\boldsymbol{\alpha}^*|^2}}, \frac{\alpha_3^*}{\sqrt{1+|\boldsymbol{\alpha}^*|^2}}, \frac{\alpha_4^*}{\sqrt{1+|\boldsymbol{\alpha}^*|^2}}\right) = \mathbf{0}. \tag{12}$$

After determining $\boldsymbol{\alpha}^*$, the desired quaternion is now reconstructed according to

$$\bar{\eta}^* = \frac{1}{\sqrt{1+|\boldsymbol{\alpha}^*|^2}}\begin{bmatrix} 1 \\ \boldsymbol{\alpha}^* \end{bmatrix}. \tag{13}$$

Similar operations are executed in the cases that η_2 or η_3 is divided out, leading to equations for the related quantities, $\boldsymbol{\beta}^*$ and $\boldsymbol{\gamma}^*$, respectively. These are one example of the four algorithms which arise for computing $\bar{\eta}^*$. Because of the quaternion norm condition, equation (2), one component must be at least 1/2 in magnitude. Therefore, one of these four algorithms must yield a quaternion which is numerically acceptable.

Such a program, though workable, is necessarily very complicated since four separate systems of equations are developed. It must be emphasized, however, that the singularity of $\boldsymbol{\rho}$ is not an indication of poor behavior on the part of the quaternion, which is generally trouble-free (in contradistinction to the Rodrigues vector and the frequently troublesome Euler angles). Nor are the complexities associated solely with the explicit intermediate solution in terms of the Rodrigues vectors, as shown, for example, by the four equations for the computation of the quaternion from the direction-cosine matrix (see Application 2 below). In one documented case, general eigenvalue methods applied to attitude determination problems that have claimed to be free of this complexity [10] can be shown, nonetheless, to have simply transferred this complexity to a different segment of the problem [11], in that case the initial condition. Thus, the need to develop four sets of equations for the quaternion seems unavoidable.

The present work develops a simple efficient procedure for obtaining all four sets of equations for generating the quaternion once one set is available which is well behaved for one of the elements of $\bar{\eta}$ not close to zero. For the example above, this method effectively obtains the equations for the three "nonstandard" Rodrigues vectors, $\boldsymbol{\alpha}^*$, $\boldsymbol{\beta}^*$, and $\boldsymbol{\gamma}^*$, once a method has been developed for determining $\boldsymbol{\rho}^*$ when η_4^* is very different from zero. It accomplishes this feat not by truly deriving four sets of equations but by interposing in the calculation simple transformations which allow the algorithm for $\boldsymbol{\rho}$ to be used for all four cases.

Sequential Rotation Theorem

Before developing a well-behaved method for solving for the quaternion, we examine a useful theorem on rotations. Consider rotations through π radians about the coordinate axes, $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$, and $\hat{\mathbf{e}}_3$

$$R(\hat{\mathbf{e}}_1,\pi) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad R(\hat{\mathbf{e}}_2,\pi) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$R(\hat{\mathbf{e}}_3,\pi) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{14}$$

and define three proper orthogonal matrices, $A^{(i)}$, $i = 1, 2, 3$, according to

$$A = A^{(1)}R(\hat{\mathbf{e}}_1,\pi), \qquad A = A^{(2)}R(\hat{\mathbf{e}}_2,\pi), \quad \text{and} \quad A = A^{(3)}R(\hat{\mathbf{e}}_3,\pi), \tag{15}$$

so that $A^{(i)}$, $i = 1,2,3$, is the "surplus attitude matrix" following a prior rotation through π about one of the three coordinate axes.[3] The near-vanishing of η_4 is the result of the angle of rotation that characterizes A being close to π. The following claim is now made:

Theorem (Sequential Rotations)

Given the three $A^{(i)}$, $i = 1,2,3$, defined above and $A^{(4)} \equiv A$, the angle of rotation of at least one of these four rotation matrices must be less than or equal to $2\pi/3$.

[3]Generally, we use A to designate the attitude matrix and R to designate any rotation matrix.

The proof is as follows: If R is an arbitrary rotation matrix, then θ, the angle of rotation characterizing R, satisfies

$$1 + 2\cos\theta = \operatorname{tr} R \equiv R_{11} + R_{22} + R_{33}, \tag{16}$$

so that the angle of rotation is a monotonically decreasing function of tr R. If tr $A^{(4)} = \operatorname{tr} A \geq 0$, then $\theta^{(4)} \leq 2\pi/3$, and the theorem is proved. Suppose, on the other hand, that tr $A < 0$. Consider then the equations for the $\theta^{(i)}$, $i = 1,2,3$, defined according to

$$1 + 2\cos\theta^{(1)} = \operatorname{tr} A^{(1)} = A_{11} - A_{22} - A_{33}, \tag{17a}$$

$$1 + 2\cos\theta^{(2)} = \operatorname{tr} A^{(2)} = -A_{11} + A_{22} - A_{33}, \tag{17b}$$

$$1 + 2\cos\theta^{(3)} = \operatorname{tr} A^{(3)} = -A_{11} - A_{22} + A_{33}. \tag{17c}$$

It is sufficient to show that at least one of the three remaining traces is nonnegative. Let A_{ii}, A_{jj}, and A_{kk} denote the three diagonal elements of A ordered such that

$$A_{ii} \geq A_{jj} \geq A_{kk}. \tag{18}$$

if tr A is negative, it follows that at least one diagonal element of A must be negative. Thus, $A_{kk} < 0$, and

$$A_{ii} > A_{jj} + A_{kk}. \tag{19}$$

Therefore,

$$A_{ii} - A_{jj} - A_{kk} > 0, \tag{20}$$

which is equivalent to

$$\operatorname{tr} A^{(i)} > 0. \tag{21}$$

This completes the proof.[4]

That $2\pi/3$ is the limiting value one can ensure for one of the four angles of rotation can be seen by examining the proper orthogonal matrix

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \tag{22}$$

for which

$$\operatorname{tr} A^{(i)} = 0, \qquad i = 1, \ldots, 4. \tag{23}$$

Note that the condition that at least one of the angles of rotation be no greater than $2\pi/3$ is equivalent to the condition that at least one component of the quaternion be no less than 1/2. This follows from the fact that tr $A^{(i)} \geq 0$ implies.

$$|\eta_4^{(i)}| = \frac{1}{2}\sqrt{1 + \operatorname{tr} A^{(i)}} \geq \frac{1}{2}. \tag{24}$$

We shall see below (from equation (32)) that equation (24) is equivalent to

$$|\eta_i| \geq 1/2. \tag{25}$$

[4]Note that Shuster and Oh [12] state incorrectly that, by sequential rotations, the angle of rotation in the computations can be made less than or equal to $\pi/2$. This error, fortunately, is not significant for the development of the algorithm derived there.

The Method of Sequential Rotations

The importance of the above result derives from the fact that an attitude problem in A can be transformed easily into an attitude problem in the $A^{(i)}$, $i = 1, 2, 3$. This transformation is generally much less burdensome than obtaining the four algorithms as in the case of the solution of equation (7b). Thus, rather than develop four different algorithms for the attitude matrix A, or attitude quaternion $\bar{\eta}$, one transforms the original problem using one of the three rotation matrices given in equation (14) and obtains four different functions $\mathbf{F}^{(i)}$, $i = 1, \ldots, 4$, where

$$\mathbf{F}^{(i)}(A) \equiv \mathbf{F}(AR(\hat{\mathbf{e}}_i, \pi)), \qquad i = 1, 2, 3, \quad \text{and} \quad \mathbf{F}^{(4)}(A) \equiv \mathbf{F}(A) . \tag{26}$$

The solution of the equations

$$\mathbf{F}^{(i)}(A) = \mathbf{0}, \qquad i = 1, \ldots, 4, \tag{27}$$

or, equivalently,

$$\mathbf{f}^{(i)}(\bar{\eta}) = \mathbf{0}, \qquad i = 1, \ldots, 4, \tag{28}$$

leads to four corresponding $A^{(i)}$, $i = 1, \ldots, 4$, or $\bar{\eta}^{(i)}$, $i = 1, \ldots, 4$, respectively, each obtained by applying the identical algorithm to each of the transformed problems.[5] Since the function $\mathbf{F}(A)$ is usually a simple construct based on vectors, and since the rotation through π about a coordinate axis only changes the signs of two components of a vector, the transformation can usually be incorporated with little effort into the function $\mathbf{F}(A)$. In fact, in estimation problems $\mathbf{F}(A)$ is generally constructed from vector data and the transformed function can then be obtained by applying the pre-rotation to the data. Thus, it is typically the data which is transformed rather than the algorithm.

By the Sequential Rotation Theorem, the quaternion associated with at least one of the $\bar{\eta}^{*(i)}$, $i = 1, \ldots, 4$, must have a scalar component which is far from zero. It is then a simple manner, once $\bar{\eta}^{*(i)}$ has been determined, to transform the computed quaternion back to $\bar{\eta}^*$.

To reconstruct $\bar{\eta}$ from one of the $\bar{\eta}^{(i)}$, $i = 1, 2, 3$, we note that for each of the three rotations through π about the three coordinate axes, the related quaternion is given by

$$\bar{\eta}(\hat{\mathbf{e}}_1, \pi) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad \bar{\eta}(\hat{\mathbf{e}}_2, \pi) = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \text{and} \quad \bar{\eta}(\hat{\mathbf{e}}_3, \pi) = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \tag{29}$$

respectively, and the surplus quaternions, which correspond to each of the surplus attitude matrices, satisfy, in similar fashion to the surplus attitude matrices,

$$\bar{\eta} = \bar{\eta}^{(1)} \otimes \bar{\eta}(\hat{\mathbf{e}}_1, \pi), \qquad \bar{\eta} = \bar{\eta}^{(2)} \otimes \bar{\eta}(\hat{\mathbf{e}}_2, \pi), \quad \text{and} \quad \bar{\eta} = \bar{\eta}^{(3)} \otimes \bar{\eta}(\hat{\mathbf{e}}_3, \pi) , \tag{30}$$

[5]Since the computation of the direction-cosine matrix directly from equation (27), if this were possible, would not lead to singularity problems, it is for the solution of equation (28) that the Method of Sequential Rotations is intended.

where $\otimes$ denotes quaternion composition, which is given by

$$\bar{\eta}' \otimes \bar{\eta} = \begin{bmatrix} \eta_4 \eta' + \eta_4' \eta - \eta' \times \eta \\ \eta_4' \eta_4 - \eta' \cdot \eta \end{bmatrix}. \tag{31}$$

Evaluating the quaternion products, the desired quaternion $\bar{\eta}$, is reconstructed from any of the surplus quaternions according to

$$\bar{\eta} = \begin{bmatrix} \eta_4^{(1)} \\ -\eta_3^{(1)} \\ \eta_2^{(1)} \\ -\eta_1^{(1)} \end{bmatrix} = \begin{bmatrix} \eta_3^{(2)} \\ \eta_4^{(2)} \\ -\eta_1^{(2)} \\ -\eta_2^{(2)} \end{bmatrix} = \begin{bmatrix} -\eta_2^{(3)} \\ \eta_1^{(3)} \\ \eta_4^{(3)} \\ -\eta_3^{(3)} \end{bmatrix}. \tag{32}$$

This method has been applied previously to optimal attitude estimation [12].

In the method outlined in the introduction, the transformation of the attitude problem by prior rotation through π about the three coordinate axes, the solution for $\bar{\eta}^{(i)}$ via $\boldsymbol{\rho}^{(i)}$, and, finally, the inverse transformation of the quaternion are equivalent to computing the quaternion from either $\boldsymbol{\rho}$, $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, or $\boldsymbol{\gamma}$. For example, the rotation through π about the $\hat{\mathbf{e}}_1$ axis, leads equivalently to an algorithm for $\boldsymbol{\alpha}^*$.

Note that although the above discussion has formulated the attitude problem in terms of the $A^{(i)}$, $i = 1, \ldots, 4$, there is no requirement that the attitude matrix ever be computed as an intermediate quantity. Nor need one necessarily always formulate the problem in terms of $\rho^{(i)}$, $i = 1, \ldots, 4$, or solve for these quantities.

Applications

To illustrate the application of the Method of Sequential Rotations to attitude problems we consider first least-squares attitude determination. The Method of Sequential Rotations has been applied previously to the QUEST algorithm [12]. We illustrate its application here to the Y-algorithm of Davenport [13], in which the problem of singularity was not considered, although it is certainly present. We derive Davenport's Y-algorithm as well in a manner much simpler than originally presented.

As a second example we examine the problem of computing the quaternion from the direction-cosine matrix. This ground has been tread many times before [3–9]. From a practical standpoint it would be surprising indeed if the present technique had anything to add. It is interesting to note, however, that the method of sequential rotations leads to Shepperd's algorithm [6], the most robust and efficient of the algorithms developed to date.

Application 1: Least-Squares Attitude Determination

A simple example of least-squares attitude estimation is the problem of determining the optimal attitude that minimizes the cost function [12–14]

$$J(A) = \frac{1}{2} \sum_{k=1}^{n} a_k |\hat{\mathbf{W}}_k - A\hat{\mathbf{V}}_k|^2, \tag{33}$$

where the a_k are a set of positive weights that satisfy

$$\sum_{k=1}^{n} a_k = 1 . \tag{34}$$

This cost function may be written equivalently as

$$J(A) = 1 - \sum_{k=1}^{n} a_k \hat{\mathbf{W}}_k \cdot A\hat{\mathbf{V}}_k \tag{35}$$

$$= 1 - \operatorname{tr}(B^T A) , \tag{36}$$

where

$$B \equiv \sum_{k=1}^{n} a_k \hat{\mathbf{W}}_k \hat{\mathbf{V}}_k^T . \tag{37}$$

If equation (3) is now substituted into equation (36), the cost function assumes the form

$$J(\bar{\eta}) \equiv J(A(\bar{\eta})) = 1 - [\boldsymbol{\eta}^T(S - sI_{3\times3})\boldsymbol{\eta} + 2\eta_4 \mathbf{Z}^T\boldsymbol{\eta} + s\eta_4^2] , \tag{38}$$

where

$$S \equiv B + B^T, \qquad s \equiv \operatorname{tr} B, \quad \text{and} \quad \mathbf{Z} \equiv \begin{bmatrix} B_{23} - B_{32} \\ B_{31} - B_{13} \\ B_{12} - B_{21} \end{bmatrix} . \tag{39}$$

In terms of the Rodrigues vector the cost function becomes finally

$$J(\boldsymbol{\rho}) \equiv J(\bar{\eta}(\boldsymbol{\rho})) = 1 - (1 + |\boldsymbol{\rho}|^2)^{-1}[\boldsymbol{\rho}^T(S - sI_{3\times3})\boldsymbol{\rho} + 2\mathbf{Z}^T\boldsymbol{\rho} + s] , \tag{40}$$

which may be minimized over $\boldsymbol{\rho}$, leading straightforwardly to the equation

$$[\boldsymbol{\rho}^{*T}(S - sI_{3\times3})\boldsymbol{\rho}^* + 2\mathbf{Z}^T\boldsymbol{\rho}^* + s]\boldsymbol{\rho}^* - (1 + |\boldsymbol{\rho}^*|^2)[(S - sI_{3\times3})\boldsymbol{\rho}^* + \mathbf{Z}] = \mathbf{0} . \tag{41}$$

Equation (41) is somewhat forbidding. A simplification of terms can be obtained by taking the scalar product of equation (41) with $\boldsymbol{\rho}^*$, which leads to

$$\boldsymbol{\rho}^{*T}(S - sI_{3\times3})\boldsymbol{\rho}^* = |\boldsymbol{\rho}^*|^2 s - (1 - |\boldsymbol{\rho}^*|^2)\mathbf{Z}^T\boldsymbol{\rho}^* . \tag{42}$$

Substituting this into equation (41) leads to the simpler equation [13]

$$[S - (\mathbf{Z}^T\boldsymbol{\rho}^* + 2s)I_{3\times3}]\boldsymbol{\rho}^* + \mathbf{Z} = \mathbf{0} , \tag{43}$$

which may be solved formally to yield

$$\boldsymbol{\rho}^* = [(\mathbf{Z}^T\boldsymbol{\rho}^* + 2s)I_{3\times3} - S]^{-1}\mathbf{Z} . \tag{44}$$

The desired value of the Rodrigues vector can be evaluated by repeated substitution. For this algorithm to be efficient, however, a good starting value of $\mathbf{Z}^T\boldsymbol{\rho}^*$ must be available. To obtain such a starting value, note that substitution of equation (42) into equation (38) leads to

$$J(\boldsymbol{\rho}^*) = 1 - \mathbf{Z}^T\boldsymbol{\rho}^* - s . \tag{45}$$

Hence,

$$\mathbf{Z}^{\mathrm{T}}\boldsymbol{\rho}^* = 1 - s - J(\boldsymbol{\rho}^*)$$
$$\approx 1 - s, \tag{46}$$

which provides the desire starting value.[6] Equation (44) was first derived by Davenport [13] and called by him the *Y-algorithm* (because he used **Y** rather than $\boldsymbol{\rho}$ to denote the Rodrigues vector).

Having developed the algorithm for $\boldsymbol{\rho}$, it would be extremely burdensome (and a significant source of human error) to reformulate the problem in terms of $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ in the manner described in the introduction. In particular, the parameterizations of equation (39) in terms of scalars, vectors and 3×3 matrices constructed in a natural manner from B would be lost. However, it is readily apparent that these equations can be obtained equivalently by solving for $\boldsymbol{\rho}^{(i)}$, $i = 1,2,3$, obtained by transforming $J(\boldsymbol{\rho})$, which is accomplished by transforming the $\hat{\mathbf{V}}_k$ according to the method of sequential rotations

$$\hat{\mathbf{V}}_k^{(i)} \equiv R(\hat{\mathbf{e}}_i, \pi)\hat{\mathbf{V}}_k, \qquad k = 1,\ldots,n, \qquad i = 1,2,3. \tag{47}$$

These transformations of the vectors are equivalent to computing new $S^{(i)}$, $\mathbf{Z}^{(i)}$, and $s^{(i)}$, $i = 1,2,3$, from

$$B^{(i)} \equiv BR(\hat{\mathbf{e}}_i, \pi), \qquad i = 1,2,3. \tag{48}$$

The multiplication by $R(\hat{\mathbf{e}}_i, \pi)$ simply changes the signs of two columns of B. The Rodrigues vector for the transformed problems is solved in each case using equation (44) but with the transformed matrix $B^{(i)}$. The solution for the Euler-Rodrigues symmetric parameters for each of the transformation is then given by equation (32). Thus, the derivation of three new algorithms is replaced by a few changes of sign.

Application 2: Quaternion Extraction

As a second example of this geometric approach, consider the problem of extracting the quaternion from the direction-cosine matrix [3–9]. The most efficient method is that published by Shepperd [6], in which the quaternion is computed from one of the following sets of equations:

$$\eta_4 = \frac{1}{2}\sqrt{1 + A_{11} + A_{22} + A_{33}}, \qquad \eta_1 = \frac{1}{4\eta_4}(A_{23} - A_{32}),$$
$$\eta_2 = \frac{1}{4\eta_4}(A_{31} - A_{13}), \qquad \eta_3 = \frac{1}{4\eta_4}(A_{12} - A_{21}), \tag{49}$$

$$\eta_1 = \frac{1}{2}\sqrt{1 + A_{11} - A_{22} - A_{33}}, \qquad \eta_2 = \frac{1}{4\eta_1}(A_{12} + A_{21}),$$
$$\eta_3 = \frac{1}{4\eta_1}(A_{13} + A_{31}), \qquad \eta_4 = \frac{1}{4\eta_1}(A_{23} - A_{32}), \tag{50}$$

[6] Shuster and Oh [12] employed a somewhat more sophisticated method to determine the least-squares attitude, which equivalently lead to this starting value for $\mathbf{Z}^{\mathrm{T}}\boldsymbol{\rho}^*$. This method also provided a discriminator, which could determine the necessity and the suitability of a prior rotation before the quaternion was actually computed.

$$\eta_2 = \frac{1}{2}\sqrt{1 - A_{11} + A_{22} - A_{33}}, \qquad \eta_1 = \frac{1}{4\eta_2}(A_{21} + A_{12}),$$

$$\eta_3 = \frac{1}{4\eta_2}(A_{23} + A_{32}), \qquad \eta_4 = \frac{1}{4\eta_2}(A_{31} - A_{13}), \tag{51}$$

$$\eta_3 = \frac{1}{2}\sqrt{1 - A_{11} - A_{22} + A_{33}}, \qquad \eta_1 = \frac{1}{4\eta_3}(A_{31} + A_{13}),$$

$$\eta_2 = \frac{1}{4\eta_3}(A_{32} + A_{23}), \qquad \eta_4 = \frac{1}{4\eta_3}(A_{12} - A_{21}). \tag{52}$$

One evaluates that set of equations for which the argument of the square root is largest, or, equivalently, as shown by Shepperd [6], according to whether tr A, A_{11}, A_{22}, or A_{33}, respectively, is largest.

Shepperd's algorithm, it turns out, follows directly from the method of sequential rotations. To see that his method is equivalent to the first set of equations, equation (49), augmented by the method of sequential rotations, let us apply a rotation about $\hat{\mathbf{e}}_1$ to A and examine the expression for the quaternion obtained using $A^{(1)}$ as an intermediate argument. Thus, we compute the intermediate quaternion, $\bar{\eta}^{(1)}$, corresponding to

$$A^{(1)} = \begin{bmatrix} A_{11} & -A_{12} & -A_{13} \\ A_{21} & -A_{22} & -A_{23} \\ A_{31} & -A_{32} & -A_{33} \end{bmatrix}. \tag{53}$$

Recalling equation (32)

$$\eta_1 = \eta_4^{(1)} = \frac{1}{2}\sqrt{1 + \text{tr}\, A^{(1)}}$$

$$= \frac{1}{2}\sqrt{1 + A_{11} - A_{22} - A_{33}}, \tag{54a}$$

$$\eta_2 = -\eta_3^{(1)} = -\frac{1}{4\eta_4^{(1)}}(A_{12}^{(1)} - A_{21}^{(1)})$$

$$= \frac{1}{4\eta_1}(A_{12} + A_{21}), \tag{54b}$$

$$\eta_3 = \eta_2^{(1)} = \frac{1}{4\eta_4^{(1)}}(A_{31}^{(1)} - A_{13}^{(1)})$$

$$= \frac{1}{4\eta_1}(A_{13} + A_{31}), \tag{54c}$$

$$\eta_4 = -\eta_1^{(1)} = -\frac{1}{4\eta_4^{(1)}}(A_{23}^{(1)} - A_{32}^{(1)})$$

$$= \frac{1}{4\eta_1}(A_{23} - A_{32}), \tag{54d}$$

which is the same as equation (50). Equations (51) and (52) follow in a similar manner from the computation of $\bar{\eta}^{(2)}$ and $\bar{\eta}^{(3)}$, respectively.

Discussion

The utility of the method of sequential rotations is that it eliminates the need to construct four substantially different versions of an algorithm for computing the quaternion in order to avoid the loss of significance resulting from the near vanishing of a quaternion component. Stated in other terms, it presents a simple paradigm for constructing the four versions of a quaternion computation algorithm. Thus, once an algorithm is available which is trouble-free when η_4 is very different from zero, the method of sequential rotations automatically produces the algorithm for the associated cases in which η_1, η_2, or η_3 is different than zero. The arithmetical operations required by this method are generally much simpler than deriving all four algorithms individually in a manner similar to that presented in the introduction. The prior multiplication of the attitude matrix by a rotation matrix for a rotation through π about one of the coordinate axes can be accomplished simply, in this case by changing the signs of two of the columns of A or two columns or rows of some related matrix in the problem. The reconstruction of the quaternion likewise can be accomplished by only two sign changes and a reordering of the components. The need to use such a construction is not always present. However, in cases where an estimate of the quaternion must be computed without prior knowledge, and, hence, it cannot be known *ab initio* that a single algorithm will yield a numerically acceptable result, this method is less burdensome, certainly, than computing one or more sets of Euler angles or separately deriving solutions for each of the four varieties of the Rodrigues vector.

An interesting by-product of this work is that the four related algorithms for extracting the quaternion from a direction-cosine matrix can be understood geometrically, essentially by referring the quaternion to one of four intermediate reference frames, rather than just as a numerical trick to avoid the singularity of the square-root function. Shepperd's algorithm is sufficiently simple that the four algorithms can be derived explicitly and this is supposedly the path followed by Shepperd [6]. Most attitude problems (for example, Application 1) cannot be so easily treated.

Unfortunately, the method of sequential rotations does not provide the means for determining which of the four algorithms is preferred. The figure of merit for determining the best of the four algorithms must come from the single algorithm to which the method of sequential rotations is applied. Very often the numerical difficulty one seeks to avoid appears as a division by a number close to zero. One therefore tests this quantity for each of the four algorithms or simply applies the four pre-rotations (including the null rotation) until an acceptable value for the divisor is found. This is the approach of the QUEST algorithm [12], to which the method of sequential rotations was first applied.

Conclusions

It has been demonstrated that although the quaternion is a nonsingular representation of the attitude, nonetheless practical solutions for the quaternion are generally singular and the singularity is avoided generally by choosing one of four possible algorithms for calculating the quaternion. These four algorithms are formally identical (within an overall sign) but have differing numerical properties. At least one of these algorithms will always be well behaved numerically. A simple geometrically-based methodology has been developed for obtaining all four algorithms for calculating the quaternion once one (possibly singular) algorithm is known. As examples of the application of this methodology we have considered least-squares estimation of the quaternion from vector data and the extraction of the quaternion from the rotation matrix. In the latter application we show that the proposed methodology leads directly to Shepperd's algorithm, the most efficient and best behaved numerically of the current algorithms for calculating the quaternion from the rotation matrix.

Acknowledgment

The authors are grateful to James Keat and F. Landis Markley for helpful criticisms. One of the authors (G. A. N.) was supported by NASA Goddard Space Flight Center under contract NAS 5-31500. The encouragement and support of Francis E. McGarry and Thomas H. Stengle of the Flight Dynamics Division of NASA Goddard Space Flight Center are gratefully acknowledged.

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