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Engineering Notes

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Unit Quaternion from Rotation Matrix

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Introduction

It is well known that a 3×3 proper orthogonal rotation matrix, or attitude matrix, can be expressed in terms of a quaternion

$$\mathbf{q} = [q_1 \quad q_2 \quad q_3 \quad q_4]^T \tag{1}$$

as [1,2]

$$A = \begin{bmatrix} q_1^2 - q_2^2 - q_3^2 + q_4^2 & 2(q_1q_2 + q_3q_4) & 2(q_1q_3 - q_2q_4) \\ 2(q_1q_2 - q_3q_4) & -q_1^2 + q_2^2 - q_3^2 + q_4^2 & 2(q_2q_3 + q_1q_4) \\ 2(q_1q_3 + q_2q_4) & 2(q_2q_3 - q_1q_4) & -q_1^2 - q_2^2 + q_3^2 + q_4^2 \end{bmatrix} \tag{2}$$

where the quaternion is assumed to have unit norm

$$\|\mathbf{q}\|^2 \triangleq \mathbf{q}^T\mathbf{q} = q_1^2 + q_2^2 + q_3^2 + q_4^2 = 1 \tag{3}$$

Often one must find the quaternion corresponding to a given rotation matrix. Of the many methods that have been proposed for performing this computation [3–9], Shepperd's algorithm [5], which is singularity free and requires only one square root, has been the most widely applied. In this Note, we review Shepperd's algorithm and present a variant that always produces a normalized quaternion even if numerical errors cause the matrix A to be only approximately orthogonal. This modification of Shepperd's algorithm also provides a very efficient method for computing an exactly orthogonal matrix that is close to an approximately orthogonal matrix.

Shepperd's Algorithm

The following relations for all the products of two quaternion components are easily derived from Eqs. (2) and (3):

$$4q_i^2 = 1 + A_{ii} - A_{jj} - A_{kk} = 1 - \mathrm{tr}A + 2A_{ii} \tag{4a}$$

$$4q_4^2 = 1 + A_{11} + A_{22} + A_{33} = 1 - \mathrm{tr}A + 2\,\mathrm{tr}A \tag{4b}$$

$$4q_iq_j = A_{ij} + A_{ji} \tag{4c}$$

$$4q_iq_4 = A_{jk} - A_{kj} \tag{4d}$$

where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$, and $\mathrm{tr}A$ denotes the trace of A. Shepperd's algorithm first compares the right sides of Eqs. (4a) and (4b) to see which of the quantities q_i^2 for $i = 1, 2, 3, 4$ is largest. The unusual form of expressing the rightmost member of Eq. (4b) shows that this is equivalent to finding the largest of $\mathrm{tr}A$ and A_{ii}, saving some computation. Note that all the quantities $4q_i^2$ are positive, and that Eq. (3) or Eqs. (4a) and (4b) show that they sum to 4. Thus, at least one of the right-hand sides of Eqs. (4a) and (4b) must be greater than or equal to unity.

In the case that q_4^2 is larger than any of the other q_i^2, Shepperd's algorithm computes q_4 from Eq. (4b) and the other components from Eq. (4d), giving

$$q_4 = \pm\tfrac{1}{2}(1 + A_{11} + A_{22} + A_{33})^{1/2} \tag{5a}$$

$$q_i = (A_{jk} - A_{kj})/4q_4 \quad \text{for } i = 1, 2, 3 \tag{5b}$$

We observe the well-known twofold sign ambiguity in the quaternion. If q_i for $i \neq 4$ is the largest quaternion component in magnitude, it is computed from Eq. (4a) and the other quaternion components are computed from Eqs. (4c) and (4d), giving

$$q_i = \pm\tfrac{1}{2}(1 + A_{ii} - A_{jj} - A_{kk})^{1/2} \tag{6a}$$

$$q_j = (A_{ij} + A_{ji})/4q_i \tag{6b}$$

$$q_k = (A_{ik} + A_{ki})/4q_i \tag{6c}$$

$$q_4 = (A_{jk} - A_{kj})/4q_i \tag{6d}$$

where $\{i, j, k\}$ is a cyclic permutation of $\{1, 2, 3\}$ as before. Shuster and Natanson have commented on the relation between the four possible branches in Shepperd's algorithm and the method of sequential rotations [10]. Shepperd's algorithm is guaranteed to produce a precisely normalized quaternion only if A is precisely orthogonal.

Modification of Shepperd's Algorithm

For the modification of Shepperd's algorithm, we consider the four 4-component vectors

$$\mathbf{x}^{(i)} \triangleq 4q_i\mathbf{q} \quad \text{for } i = 1, 2, 3, 4 \tag{7}$$

Each of the four components of each $\mathbf{x}^{(i)}$ is given by the right side of one of the equations of Eqs. (4), so these vectors are easily computable from the components of the rotation matrix. Explicitly,

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$$\mathbf{x}^{(1)} = \begin{bmatrix} 1 + A_{11} - A_{22} - A_{33} \\ A_{12} + A_{21} \\ A_{13} + A_{31} \\ A_{23} - A_{32} \end{bmatrix} \tag{8a}$$

$$\mathbf{x}^{(2)} = \begin{bmatrix} A_{21} + A_{12} \\ 1 + A_{22} - A_{33} - A_{11} \\ A_{23} + A_{32} \\ A_{31} - A_{13} \end{bmatrix} \tag{8b}$$

$$\mathbf{x}^{(3)} = \begin{bmatrix} A_{31} + A_{13} \\ A_{32} + A_{23} \\ 1 + A_{33} - A_{11} - A_{22} \\ A_{12} - A_{21} \end{bmatrix} \tag{8c}$$

$$\mathbf{x}^{(4)} = \begin{bmatrix} A_{23} - A_{32} \\ A_{31} - A_{13} \\ A_{12} - A_{21} \\ 1 + A_{11} + A_{22} + A_{33} \end{bmatrix} \tag{8d}$$

Equation (7) shows that each of the $\mathbf{x}^{(i)}$ is a scalar multiple of $\mathbf{q}$, so we can obtain the unit quaternion by computing and normalizing any one of the $\mathbf{x}^{(i)}$

$$\mathbf{q} = \pm \mathbf{x}^{(i)} / \|\mathbf{x}^{(i)}\| \tag{9}$$

As in Shepperd's method, choosing the $\mathbf{x}^{(i)}$ corresponding to the maximum value of q_i^2 minimizes numerical errors. This selection is made by Shepperd's procedure of finding the largest of tr$A$ and A_{ii}.

This method of extracting a quaternion from a rotation matrix requires the same number of square roots as Shepperd's method, namely one, but one more division and a few more additions and multiplications. A slightly modified form of this method was previously used to extract a quaternion from a scalar multiple of the attitude matrix [11].

Orthogonalization

Strapdown inertial systems often employ the numerical integration of a rotation matrix that can lose orthogonality due to accumulation of roundoff error. Various methods have been proposed to restore orthogonality, some approximate or iterative and often requiring matrix inversion [12–14]. Equations (8) and (9) provide an exact (within machine precision) noniterative method for restoring orthogonality by simply substituting the result of Eq. (9) into Eq. (2) to produce a new matrix A_{orth}. The normalization condition of Eq. (3) guarantees that A_{orth} is orthogonal. Because Eq. (2) is a homogenous quadratic function of $\mathbf{q}$, the square root in Eq. (9) can be avoided if we only need to compute A_{orth} and not $\mathbf{q}$; the matrix elements of A_{orth} are rational functions of the matrix elements of A. This computation is much less expensive than any previously proposed for orthogonalization.

Conclusions

It is interesting to see how well this procedure recovers an orthogonal matrix from a rotation matrix corrupted by computational errors. The computational errors are modeled as independent random numbers uniformly distributed in $[\varepsilon, -\varepsilon]$ added to each component of the true rotation matrix. The measure of performance is the rotation angle vector $\boldsymbol{\theta}$ representing the rotation from A_{orth} to the true rotation matrix. Numerical simulation or analysis to lowest nonzero order in ε shows that $\boldsymbol{\theta}$ has zero mean and that the expectation of $|\boldsymbol{\theta}|^2$ is $(7q_i^{-2} - 1)\varepsilon^2/12$ rad^2, where q_i is the quaternion component on the right side of Eq. (7) corresponding to the particular instance of Eqs. (8a–8d) used to compute the quaternion. This is the component having the largest magnitude, and the quaternion normalization condition of Eq. (3) ensures that $1 \le q_i^{-2} \le 4$. This shows the importance of choosing the $\mathbf{x}^{(i)}$ corresponding to the maximum value of q_i^2; otherwise the errors could be unbounded. With the optimal choice, the standard deviation of the attitude error, the square root of the expectation of $|\boldsymbol{\theta}|^2$, will be between $\varepsilon/\sqrt{2}$ and $3\varepsilon/2$ rad. Averaging the expectation of $|\boldsymbol{\theta}|^2$ over uniformly distributed random rotation matrices (i.e., for quaternions uniformly distributed on the unit sphere S3 in four-dimensional space) gives an overall attitude error standard deviation of 0.964ε rad.

This method does not solve the orthogonal Procrustes problem, which finds the orthogonal matrix closest to A in the Frobenius norm, that is, the orthogonal matrix A_{orth} minimizing $\|A_{\text{orth}} - A\|_F^2$, or equivalently the quaternion minimizing $\|A(q) - A\|_F^2$, where the Frobenius norm of an $N \times N$ real matrix is defined as

$$\|M\|_F^2 = \sum_{i,j=1}^{N} M_{ij}^2$$

The solution to the Procrustes problem can be found by a modification of Shuster's quaternion estimator (QUEST) [15] or of Davenport's q method [9,16]. The latter finds the quaternion representation of the closest orthogonal matrix as the eigenvector with the largest eigenvalue of the symmetric 4×4 matrix

$$K \equiv \begin{bmatrix} A + A^T - I_{3\times 3}\,\text{tr}A & \mathbf{z} \\ \mathbf{z}^T & \text{tr}A \end{bmatrix} \tag{10}$$

where $I_{3\times 3}$ is the 3×3 identity matrix and

$$\mathbf{z} \equiv \begin{bmatrix} A_{23} - A_{32} \\ A_{31} - A_{13} \\ A_{12} - A_{21} \end{bmatrix} \tag{11}$$

Under the same assumptions on the errors in A, the standard deviation of the angular errors resulting from the Proctrustes method is $\varepsilon/\sqrt{2}$ rad independent of the true rotation matrix. We see that the Procrustes method produces a result that is somewhat closer to the truth in these random error tests, but with significantly greater computational burden. The difference between the two methods is negligible for the level of numerical errors expected in computing the attitude matrix, however. It should also be emphasized that the Procrustes method is not optimal unless the errors in A are isotropic [17].

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