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A review on non iterative closed form configuration matching and rotations estimation

M. De Agostino, C. Porporato, M. Roggero

Abstract. Orthonormal matrices, Procrustes and quaternion analysis are closed form solutions of the configuration matching problem, common in geodesy as in the datum transformation problem. Literature reports more Procrustes based geodetic applications than Quaternions, which are more used in other application fields, such as aerospace navigation, robotics and computer vision. The large popularity of Procrustes in geodesy is mainly due to its capability to take into account a priori observation weighting in a simple way.

Keywords. Rotations, quaternions, orthonormal matrices, Procrustes.

1 Introduction

A rotation is a transformation of the Euclidean space that rigidly moves objects leaving fixed at least one point (the origin of Euclidean space). In geodesy rotations are involved in many problems, especially for solving the transformation between reference frames. More in detail, a rotation is an isometry of an Euclidean space that preserves the orientation, and it is described by an orthogonal matrix. In a Euclidean space of two or three dimensions each orthogonal ma-

trix expresses a rotation around a point or an axis, a reflection, or a combination of these two transformations.

As mentioned above, the representation of a rotation expresses the orientation of an object with respect to a reference system, or the relative orientation of two or more reference systems. Euler's theorem shows that any space rotation can be decomposed into the product of the three rotations $R_\psi^i R_\theta^j R_\phi^k$, where $i \neq j \neq k$ and $i, j, k \in \mathbb{R}^3$, and where R_α^i indicates a rotation of α radians counterclockwise around the i axis. According to Euler's theorem, the attitude of a rigid body can be described by a rotation around only one axis. Furthermore, this rotation can be defined uniquely by a minimum of three parameters, such as the directors cosines matrices, that represent the most widespread method for estimating rotations into geodetic networks.

However, for various reasons, there are several ways to represent rotations, making use of a number of parameters even higher than three, although also those redundant representations have always only three degrees of freedom. Some of these methods, presented over the years, are hereinafter described and compared.

2 The Quaternion-based approach

What Sir William Rowan Hamilton wrote on the 16th of October 1843 on a stone of Brougham Bridge in Dublin, is simply:

$$i^2 = j^2 = k^2 = ijk = -1 \quad (1)$$

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Fig.1 The Brougham Bridge in Dublin and the Hamilton commemorative plaque

The combination:

$$\dot{q} = q_0 + iq_1 + jq_2 + kq_3 \quad (2)$$

where q_0, q_1, q_2 and q_3 are real numbers, defines the generic quaternion. Quaternions satisfy all the laws of algebra, except the multiplication commutative law. In fact:

$$ij = -ji, \quad jk = -kj, \quad ki = -ik \quad (3)$$

which represents a serious violation of the commutative law $ab = ba$. It is also apparent:

$$\begin{aligned} ij &= k & jk &= i & ki &= j \\ ji &= -k & kj &= -i & ik &= -j \end{aligned} \quad (4)$$

The fundamental values of quaternions, i, j and k , can be handled as three mutually perpendicular clockwise axes in a common three-dimensional Euclidean space. Each unit quaternion, in particular, define a rotation in \mathbb{R}^3 space. These rotations are given by the conjugate:

$$\dot{r}' = \dot{q}\dot{r}\dot{q}^{-1} = \dot{q}\dot{r}\dot{q}^* \quad (5)$$

It can be verified that if \dot{r} is purely imaginary (the real part is equal to zero), also \dot{r}' is purely imaginary; therefore it can be defined an action of the group of unit quaternions on \mathbb{R}^3 . Each action defined in this way is indeed a rotation, since it preserves the norm:

$$|\dot{r}'| = |\dot{q}\dot{r}\dot{q}^*| = |\dot{q}||\dot{r}||\dot{q}^*| = |\dot{r}| \quad (6)$$

It is possible to show the equivalence between the conjugate and the product of the 3x3 Rodriguez rotation matrix and a real vector. In fact, the operation:

$$\dot{q}\dot{r}\dot{q}^* = (Q\dot{r})\dot{q}^* = \bar{Q}^T(Q\dot{r}) = (\bar{Q}^T Q)\dot{r} \quad (7)$$

produce a 4x4 rotation matrix $\bar{Q}^T Q$, whose lower right 3x3 sub-matrix is orthonormal, and it is the rotation matrix that takes \dot{r} to \dot{r}' .

Given the three-dimensional rotation between two frames \dot{r} and \dot{s} with a scale-change ρ :

$$\dot{s} = \rho \dot{q}\dot{r}\dot{q}^* \quad (8)$$

where $\dot{q}\dot{q}^* = 1$, the measurement equation is:

$$\dot{v}_i = \dot{s}_i - \rho \dot{q}\dot{r}_i\dot{q}^* \quad (9)$$

where \dot{v}_i are still purely imaginary quaternions. In the following, we will present two methods in the literature to solve the problem (9), respectively by minimizing the residual vector \dot{v} (Sansò, 1973) or alternatively maximizing the scalar product $\dot{s} \cdot \dot{r}$ (Horn, 1987).

2.1 Residual vector minimization

In accordance with the least squares approach, we must compute the minimum of the function:

$$\Phi(\dot{q}, \rho) = \sum_i \dot{v}_i^* \dot{v}_i \quad (10)$$

where $|\dot{q}|^2 = \dot{q}\dot{q}^* = 1$. Differentiating Φ with respect to ρ and \dot{q} and introducing a real Lagrange multiplier α , we obtain, after some mathematical steps:

$$\left[\sum_i |\dot{s}_i|^2 + \rho^2 \sum_i |\dot{r}_i|^2 + \alpha \right] \dot{q} + 2\rho \sum_i \dot{s}_i \dot{q}\dot{r}_i = 0 \quad (11)$$

It is possible to show that:

$$\sum_i |\dot{s}_i|^2 = \rho^2 \sum_i |\dot{r}_i|^2 - \alpha \quad (12)$$

Using equation (12) in (11), through some mathematical steps we reach the final equation:

$$\begin{aligned} \left(\sum_i \dot{r}_i \dot{s}_i \right) \dot{q} &= \left(-\rho \sum_i |\dot{r}_i|^2 \right) \dot{q} \\ A\dot{q} &= \lambda \dot{q} \end{aligned} \quad (13)$$

As it is possible to see, the unknowns λ and \dot{q} are respectively an eigenvalue and eigenvector of a symmetric matrix A , that can be built directly from the data \dot{r}_i and \dot{s}_i . In particular, using the products expansion rules of quaternions, we find:

$$\begin{aligned} \sum_i \dot{r}_i \dot{s}_i \dot{q} &= \sum_i \dot{s}_i \dot{q}\dot{r}_i = \sum_i (S_i \dot{q}) \dot{r}_i = \sum_i \bar{R}_i (S_i \dot{q}) = \\ &= \left(\sum_i \bar{R}_i S_i \right) \dot{q} = \left(\sum_i A_i \right) \dot{q} \end{aligned} \quad (14)$$

from which it is possible to derive the expressions of A_i and A .

2.2 Scalar product maximization

In this second approach, we seek the quaternion \hat{q} to maximize the scalar product:

$$\sum_{i=1}^n (\hat{q}_i \hat{q}^*) \cdot \dot{s}_i = \sum_{i=1}^n \dot{r}_i' \cdot \dot{s}_i \quad (15)$$

Reminding the geometric meaning of the scalar product of vectors, we have:

$$\dot{r}_i' \cdot \dot{s}_i = |\dot{r}_i'| |\dot{s}_i| \cos \theta \quad (16)$$

where θ is the angle subtended. Since $|\dot{r}_i'| = |\dot{r}_i|$ and $|\dot{s}_i|$ are constants, the maximization of the scalar product is equal to minimize the parameter θ (or maximize $\cos \theta$). Using the above results, we can rewrite the scalar product as:

$$\sum_{i=1}^n (\hat{q}_i \dot{r}_i) \cdot (\dot{s}_i \hat{q}) \quad (17)$$

The products $(\hat{q}_i \dot{r}_i)$ and $(\dot{s}_i \hat{q})$ can be expressed by means of the matrices R and S , therefore:

$$\begin{aligned} \sum_{i=1}^n (\hat{q}_i \dot{r}_i) \cdot (\dot{s}_i \hat{q}) &= \sum_{i=1}^n \hat{q}^T \bar{R}_i^T S_i \hat{q} = \\ &= \hat{q}^T \left(\sum_{i=1}^n \bar{R}_i^T S_i \right) \hat{q} = \\ &= \hat{q}^T \left(\sum_{i=1}^n \hat{A}_i \right) \hat{q} = \hat{q}^T \hat{A} \hat{q} \end{aligned} \quad (18)$$

It is now simple to derive the values of the sub-matrices \hat{A}_i , and consequently of the matrix \hat{A} , where $\hat{A}_i^T = \hat{A}_i$ and $\hat{A}^T = \hat{A}$. Recalling that we were seeking:

$$\text{Max}_{\hat{q}} \left(\sum_{i=1}^n \dot{r}_i' \cdot \dot{s}_i \right) = \text{Max}_{\hat{q}} (\hat{q}^T \hat{A} \hat{q}) \quad (19)$$

It is possible to note that $\hat{A} = -A$.

3 The Orthonormal matrices approach

Among the existing ways to represent rotation we present one that is most often used in photogrammetry: the orthonormal matrices. Again r is the position vector in the original RS and s the position vector in the final RS. The aim is to find the rotation that minimizes the residual errors. Therefore, we have to find the orthonormal matrix B , 3×3 matrix, that maximize

$$\sum_{i=1}^n s_i (B r_i) = \sum_{i=1}^n s_i^T B r_i \quad (20)$$

Being

$$a^T B b = \text{Tr} (B^T a b^T) \quad (21)$$

it is possible to write the (20) as

$$\text{Tr} \left(B^T \sum_{i=1}^n s_i r_i^T \right) = \text{Tr} (B^T M) \quad (22)$$

where $M = \sum_{i=1}^n s_i r_i^T$ and

$$M = \begin{bmatrix} \sum_i s_i^1 r_i^1 & \sum_i s_i^1 r_i^2 & \sum_i s_i^1 r_i^3 \\ \sum_i s_i^2 r_i^1 & \sum_i s_i^2 r_i^2 & \sum_i s_i^2 r_i^3 \\ \sum_i s_i^3 r_i^1 & \sum_i s_i^3 r_i^2 & \sum_i s_i^3 r_i^3 \end{bmatrix} \quad (23)$$

It follows that the rotation that minimize the residual errors corresponds to the orthonormal matrix B that maximizes $\text{Tr} (B^T M)$.

A square matrix M could always be decomposed into the product of an orthonormal matrix U and a positive semi-definite matrix S . When M is non singular, the matrices U and S are univocally determined and it allows to write

$$M = \frac{M}{(M^T M)^{1/2}} (M^T M)^{1/2} = US \quad (24)$$

In this expression, $U = M (M^T M)^{-1/2}$ is an orthonormal matrix and $S = (M^T M)^{1/2}$ is the square root positive semi-definite of the symmetric matrix $M^T M$.

It is possible to write this matrix $M^T M$ using its eigenvalues $\{\lambda_i\}$ and eigenvectors $\{\hat{u}_i\}$ as following:

$$M^T M = \lambda_1 \hat{u}_1 \hat{u}_1^T + \lambda_2 \hat{u}_2 \hat{u}_2^T + \lambda_3 \hat{u}_3 \hat{u}_3^T \quad (25)$$

Since $M^T M$ is positive semi-definite, its eigenvalues are positive and their square root is Real and it is possible to write the symmetrical matrix S

$$S = \sqrt{\lambda_1} \hat{u}_1 \hat{u}_1^T + \sqrt{\lambda_2} \hat{u}_2 \hat{u}_2^T + \sqrt{\lambda_3} \hat{u}_3 \hat{u}_3^T \quad (26)$$

As the eigenvectors are orthogonal, it follows that $S^2 = M^T M$. This expression of the S matrix is allowed also when some eigenvectors are null. For this reason, the result is positive semi-definite instead of positive definite. If all the eigenvectors are positive, S becomes

$$S^{-1} = \frac{1}{\sqrt{\lambda_1}} \hat{u}_1 \hat{u}_1^T + \frac{1}{\sqrt{\lambda_2}} \hat{u}_2 \hat{u}_2^T + \frac{1}{\sqrt{\lambda_3}} \hat{u}_3 \hat{u}_3^T \quad (27)$$

It is useful to calculate the U matrix $U = MS^{-1} = M(M^T M)^{-1/2}$. It is possible to note that the sign of the determinant of U is the same of the determinant of M matrix. In fact

$$\det(U) = \det(MS^{-1}) = \det(M) \det(S^{-1}) \quad (28)$$

And the $\det(S^{-1})$ is positive because its eigenvalues are positive. The U matrix is a rotation when $\det(M) > 0$ and it represents a reflection if $\det(M) < 0$. It is necessary to minimize this expression $\text{Tr}(B^T M) = \det(B^T U S)$ that, substituting the expression (26) becomes

$$\begin{aligned} \text{Tr}(B^T U S) &= \frac{1}{\sqrt{\lambda_1}} \text{Tr}(B^T U \hat{u}_1 \hat{u}_1^T) + \\ &+ \frac{1}{\sqrt{\lambda_2}} \text{Tr}(B^T U \hat{u}_2 \hat{u}_2^T) + \frac{1}{\sqrt{\lambda_3}} \text{Tr}(B^T U \hat{u}_3 \hat{u}_3^T) \end{aligned} \quad (29)$$

For each X and Y matrices such that the XY and YX products are square, it follows that $\text{Tr}(XY) = \text{Tr}(YX)$ and

$$\begin{aligned} \text{Tr}(B^T U \hat{u}_i \hat{u}_i^T) &= \text{Tr}(\hat{u}_i^T B^T U \hat{u}_i) = \\ &= \text{Tr}(B \hat{u}_i U \hat{u}_i) = B \hat{u}_i U \hat{u}_i \end{aligned} \quad (30)$$

Since $\{\hat{u}_i\}$ is a unit vector and both U and B are orthogonal transformations, it is verified that $B \hat{u}_i U \hat{u}_i \leq 1$. It follows that

$$\text{Tr}(B^T U S) \leq \sqrt{\lambda_1} + \sqrt{\lambda_2} + \sqrt{\lambda_3} = \text{Tr}(S) \quad (31)$$

And there is the maximum value of $\text{Tr}(B^T U S)$ when $B^T U = I$ or $B = U$. The sought orthonormal matrix is the one that arises from the decomposition of M decomposed into the product of an orthonormal matrix and symmetric one. When M is non-singular matrix, then

$$B = M(M^T M)^{-1/2} \quad (32)$$

The presented method is a closed-form solution using orthonormal matrices and their eigenvalues-eigenvector decomposition.

4 Procrustes approach

The minimization problem known as ‘‘Procrustes’’ is the technique of matching one configuration R into another configuration S in order to produce a measure of match, by an orthogonal transformation matrix T such that the sum of squares of the residual matrix $E = RT - S$ is minimum:

$$\Phi = \text{Tr}(E^T E) = \min \quad (33)$$

Expanding the product $E^T E$, the Φ can be expressed as function of T :

$$\Phi = 2\text{Tr}(T^T R^T S) + \text{Tr}(T^T R^T R T + S^T S) \quad (34)$$

which partial derivative with respect to T is

$$\begin{aligned} \frac{\partial \Phi}{\partial T} &= 2\text{Tr}(M^T) + 2\text{Tr}(T^T R^T R) = \\ &= \text{Tr}(M T^T + R^T R) \end{aligned} \quad (35)$$

The condition $\|RT - S\|^2 = \min$ it is equivalent to $\text{Tr}(S^T R T) = \text{Tr}(M^T T) = \max$. Be UDV^T the singular value decomposition of M where $D = \text{diag}(\sigma_1, \sigma_2, \sigma_3)$, then

$$\begin{aligned} \text{Tr}(T^T U D V^T) &= \text{Tr}(V^T T^T U D) = \\ &= \text{Tr}(Z D) = \sum_i z_{ii} \sigma_i \leq \sum_i \sigma_i \end{aligned} \quad (36)$$

where $Z = V^T T^T U$, that has a maximum in $Z = I$. Finally $T = UV^T$ is the optimal rotation matrix.

5 Different Approaches comparisons

The methods that are presented in this paper are widely used in geodesy, photogrammetry, robotics and computer graphic. Here we can underline some common or different aspects for each approach.

The presented approaches differ in term of rotation representation and optimization method, while the optimization criteria is always least squares.

The two quaternion approach investigated are formally equivalent. In fact, it was shown that the two matrix A and \hat{A} defined respectively for the residual vector minimization approach and for the scalar product maximization one, are related by $\hat{A} = -A$. Moreover, it is find that these matrices depend only from the data sets: \hat{r} and \hat{s} .

The orthonormal matrix approach has been studied in a closed-form solution performed using orthonormal matrices. This method requires the computation of the square root of a symmetric matrix to solve the rotation problem.

Finally the Procrustes approach is often used in photogrammetry, in order to solve the orientation problem. When the weight (both in the data set and for each 3D component) in the transformation is introduced we are dealing with the Generalized Procrustes Analysis. It is possible to shown that the used orthonormal matrix T is equivalent to the Rodriguez matrix.

The described algorithm have been implemented in a FORTRAN90 software and numerically verified on real data examples.

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