Optimal Estimation of Three-Dimensional Rotation and Reliability Evaluation

Naoya OHTA† and Kenichi KANATANI†, Members

SUMMARY We discuss optimal rotation estimation from two sets of 3-D points in the presence of anisotropic and inhomogeneous noise. We first present a theoretical accuracy bound and then give a method that attains that bound, which can be viewed as describing the reliability of the solution. We also show that an efficient computational scheme can be obtained by using quaternions and applying renormalization. Using real stereo images for 3-D reconstruction, we demonstrate that our method is superior to the least-squares method and confirm the theoretical predictions of our theory by applying bootstrap procedure.

key words: 3-D rotation, statistical inference, theoretical accuracy bound, renormalization, stereo vision, bootstrap

1. Introduction

Determining a rotational relationship between two sets of 3-D points is an important task for 3-D object reconstruction and recognition. For example, if we use stereo vision or range sensing, the 3-D shape can be reconstructed only for visible surfaces. Hence, we need to fuse separately reconstructed surfaces into one object [2],[14]. For this task, we need to determine the rigid transformation between two sets of points. If one set is translated so that its centroid coincides with that of the other, the problem reduces to estimating a rotation.

Let \( \{ r_n \} \) and \( \{ r'_n \} \), \( \alpha = 1, ..., N \), be the sets of three-dimensional vectors before and after a rotation, respectively. A conventional method for determining the rotation is the following least squares method:

\[
\sum_{\alpha=1}^{N} |r'_\alpha - R r_\alpha|^2 \rightarrow \text{min}.
\]

In this paper, \( ||a|| \) denotes the norm of a vector \( a \).


From a statistical point of view, the above least-squares method implicitly assumes the following noise model:

- Points \( \{ r_n \} \) are observed without noise, while the rotated points \( \{ R r'_n \} \) are observed with noise \( \Delta r'_n \).
- The noise \( \{ \Delta r'_n \} \) is subject to an isotropic, identical, and independent Gaussian distribution of zero mean.

The least-squares solution is optimal for this model. However, this model is not realistic for 3-D points reconstructed by stereo vision or range sensing, since the noise is usually neither isotropic nor identical. Position uncertainty is larger along the viewing direction than in the directions perpendicular to it, and it is generally larger as the distance increases. Also, the 3-D points in both sets suffer noise; it is unreasonable to assume that noise exists only in one set.

In this paper, we first introduce a realistic noise model and present a theoretical accuracy bound, which can be evaluated independently of particular solution techniques involved. Then, we describe an estimation method that attains the accuracy bound; such a method alone can be called “optimal”. Since the solution attains the accuracy bound, we can view it as quantitatively describing the reliability of the solution; in the past, the reliability issue seems to have attracted little attention.

The optimal method turns out to be highly nonlinear. However, we show that an efficient computational scheme can be obtained by using quaternions and applying the renormalization technique proposed by Kanatani [10]. Using real stereo images for 3-D reconstruction, we demonstrate that our method is superior to the least-squares method and confirm the theoretical predictions of our theory by applying bootstrap procedure [3].

2. Theoretical Analysis

Let \( \tilde{r}_\alpha \) and \( P'_\alpha \), \( \alpha = 1, ..., N \), denote the true 3-D positions before and after a rotation, respectively, and let
$r_n$ and $r'_n$ be their respective positions observed in the presence of noise. We write

$$r_n = \hat{r}_n + \Delta r_n, \quad r'_n = \hat{r}'_n + \Delta r'_n,$$

and assume that $\Delta r_n$ and $\Delta r'_n$ are independent Gaussian random variables of mean zero. Their covariance matrices are defined by

$$V[r_n] = E[\Delta r_n \Delta r_n^T], \quad V[r'_n] = E[\Delta r'_n \Delta r'_n^T],$$

where $E[\cdot]$ denotes expectation and the superscript $^T$ denotes transpose. The problem is now formally stated as follows:

**Problem 1:** Estimate the rotation matrix $\hat{R}$ that satisfies

$$\hat{r}'_n = R\hat{r}_n, \quad \alpha = 1, \ldots, N,$$

from the noisy data $\{r_n\}$ and $\{r'_n\}$.

In practice, it is often very difficult to predict the covariance matrices $V[r_n]$ and $V[r'_n]$ precisely. In many cases, however, we can estimate their relative scales. If the 3-D positions are computed by stereo vision for example, the distribution of errors can be computed up to scale from the geometry of the camera configuration [11]. In view of this, we decompose the covariance matrices into an unknown constant $\epsilon$ and known matrices $V_0[r_n]$ and $V_0[r'_n]$ in the form

$$V[r_n] = \epsilon^2 V_0[r_n], \quad V[r'_n] = \epsilon^2 V_0[r'_n].$$

We call $\epsilon$ the noise level and $V_0[r_n]$ and $V_0[r'_n]$ the normalized covariance matrices.

The reliability of an estimator is usually evaluated by its covariance matrix. However, we cannot define the covariance matrix of a rotation in the usual sense, since a rotation is an element of the group of rotations $SO(3)$, which is a three-dimensional Lie group. Let $\hat{R}$ be an estimator of the true rotation $R$. Let $t_r$ and $\Delta \Omega$ be, respectively, the axis (unit vector) and the angle of the relative rotation $\hat{R}R^T$. We define a three-dimensional vector

$$\Delta \Omega = \Delta \Omega t_r,$$

and regard this as the measure of deviation of the estimator $\hat{R}$ from the true rotation $R$. We define the covariance matrix of $\hat{R}$ by

$$V[\hat{R}] = E[\Delta \Omega \Delta \Omega^T].$$

The group of rotations $SO(3)$ has the topology of the three-dimensional projective space $P^3$, which is locally homeomorphic to a 3-sphere $S^3$ [7]. If the noise is small, the deviation $\Delta \Omega$ is also small and identified with an element of the Lie algebra $so(3)$ of $SO(3)$. This is equivalent to regarding errors as occurring in the tangent space to the 3-sphere $S^3$ at $\hat{R}$. Hence, we can apply the theory of Kanatani (Sect. 14.4.3 of [10]) to obtain a theoretical accuracy bound, which he called the Cramer-Rao lower bound in analogy with the corresponding bound in traditional statistics. In the present case, it reduces to

$$V[\hat{R}] > \epsilon^2 \left( \sum_{n=1}^{N} (\hat{R}\hat{r}_n) \times (\hat{R}\hat{r}_n) \right)^{-1},$$

$$\hat{W}_n = (\hat{R}V_0[r_n]\hat{R}^T + V_0[r'_n])^{-1}.$$
If \( V_0[r_a] = V_0[r'_a] = I \), Eq. (11) reduces to Eq. (1). This proves that the least-squares method (1) is optimal for isotropic and identical noise, even if \( r_a \) and \( r'_a \) both contain noise. This corresponds to the result of Goryn and Hehn [4].

The unknown noise level \( \epsilon \) can be estimated a posteriori. Let \( J \) be the residual, i.e., the minimum of \( J \). Since \( J/\epsilon^2 \) is subject to a \( \chi^2 \) distribution with \( 3(N-1) \) degrees of freedom in the first order (Sect. 7.1.4 of [10]), we obtain an unbiased estimator of the squared noise level \( \epsilon^2 \) in the following form:

\[
\epsilon^2 = \frac{J}{3(N-1)}. \tag{12}
\]

The minimization (11) must be conducted subject to the constraint that \( R \) be a rotation matrix. This means we need to parameterize \( R \) appropriately and do numerical search in the parameter space. Such a technique is often inefficient because it requires evaluation of the derivatives in complicated forms. Here, we adopt a scheme called renormalization proposed by Kanatani [10]. Although it requires eigenvalue constraints, but our constraint is nonlinear, so it cannot be applied directly. In the following, we show that the constraint can be converted into a linear equation in terms of quaternions.

4. Computational Scheme

Consider a rotation of angle \( \Omega \) around axis \( l \) (unit vector). Define a scalar \( q_0 \) and a three-dimensional vector \( q_1 \) by

\[
q_0 = \cos \frac{\Omega}{2}, \quad q_1 = l \sin \frac{\Omega}{2}. \tag{13}
\]

Note that \( q_0^2 + \|q_1\|^2 = 1 \) by definition. Conversely, a scalar \( q_0 \) and a three-dimensional vector \( q_1 \) such that \( q_0^2 + \|q_1\|^2 = 1 \) uniquely determine an axis \( l \) and angle \( \Omega \) \((0 \leq \Omega < \pi)\) of a rotation. Hence, a rotation is uniquely represented by a pair \( (q_0, q_1) \), which is called a quaternion [7].

Suppose a point \( \tilde{r} \), undergoes a rotation \( R \) of angle \( \Omega \) around axis \( l \) and moves to a new position \( \tilde{r}'\). It can be seen from the geometry of rotation that the displacement \( \tilde{r}' - \tilde{r} \) and the midpoint \((\tilde{r} + \tilde{r}')/2\) are related by

\[
\tilde{r}' - \tilde{r} = 2 \tan \frac{\Omega}{2} l \times \frac{\tilde{r} + \tilde{r}'}{2}. \tag{14}
\]

Solving this for \( \tilde{r}' \) in terms of \( \tilde{r} \), we can obtain a relation equivalent to Eq. (4) expressed in terms of the angle \( \Omega \) and axis \( l \) of rotation \( R \). Hence, Eq. (14) is equivalent to Eq. (4). Multiplying Eq. (14) by \( \cos(\Omega/2) \) on both sides, we obtain after some manipulations

\[
q_0(\tilde{r}' - \tilde{r}) + (\tilde{r}' + \tilde{r}) \times q_1 = 0. \tag{15}
\]

Define a \( 3 \times 4 \) matrix \( X_a \) and a four-dimensional unit vector \( q \) by

\[
X_a = \begin{pmatrix} r'_a - r_a & (r'_a + r_a) \times I \end{pmatrix}, \tag{16}
\]

\[
q = \begin{pmatrix} q_0 \\ q_1 \end{pmatrix}, \tag{17}
\]

where the product \( a \times A \) of a vector \( a \) and a matrix \( A \) is the matrix whose columns are vector products of \( a \) and the corresponding columns of \( A \). Let \( \tilde{X}_a \) be the value of \( X_a \) obtained by replacing \( r_a \) and \( r'_a \) by \( \tilde{r} \) and \( \tilde{r}' \), respectively, in Eq. (16). Then, Eq. (15) can be expressed as a linear equation in \( q \) in the form

\[
\tilde{X}_a q = 0. \tag{18}
\]

Now the problem is to minimize Eq. (10) subject to the constraint (18). Introducing Lagrange multipliers for this constraint and eliminating \( \tilde{r} \) and \( \tilde{r}' \), we can reduce the problem to the following minimization with respect to \( q \):

\[
J = (q, Mq) \to \min. \tag{19}
\]

Here, \( M \) is a \( 4 \times 4 \) matrix defined by

\[
M = \sum_{a=1}^{N} X_a^T W_a X_a, \tag{20}
\]

where \( W_a \) is a \( 3 \times 3 \) matrix given by

\[
W_a = (q_0^2 (V_0[r_a] + V_0[r'_a])) - 2q_0 S[q_1 \times (V_0[r_a] - V_0[r'_a])] + q_1 \times (V_0[r_a] + V_0[r'_a]) \times q_1 \quad ^{-1}. \tag{21}
\]

Here, the operation \( S[\cdot] \) designates symmetrization: \( S[A] = (A + A^\top)/2 \).

If noise is isotropic and identical, Eq. (19) reduces to the method implied by Zhang and Faugeras [17] and Weng et al. [16]. In this sense, Eq. (19) can also be viewed as an extension of their methods to cope with anisotropic noise.

Since the constraint (18) is linear, the renormalization technique of Kanatani [10] can be applied to the optimization (19). In order to do so, we first evaluate the bias of the moment matrix \( M \) defined by Eq. (20). Let \( \Delta X_a \) be the true value of \( X_a \) given by Eq. (16). If we write \( X_a = \tilde{X}_a + \Delta X_a \), the error term \( \Delta X_a \) is given by

\[
\Delta X_a = \begin{pmatrix} \Delta r'_a - \Delta r_a & (\Delta r'_a + \Delta r_a) \times I \end{pmatrix}. \tag{22}
\]

Similarly, let \( \Delta M \) be the true value of \( M \) given by Eq. (20), and write \( M = \tilde{M} + \Delta M \). Substituting
Eq. (22) into this, we see that the error term $\Delta M$ has the following expression:

$$\Delta M = \sum_{\alpha=1}^{N} \left( \Delta X_{\alpha}^\top W_{\alpha} X_{\alpha} + X_{\alpha}^\top W_{\alpha} \Delta X_{\alpha} \right) + \Delta X_{\alpha}^\top W_{\alpha} \Delta X_{\alpha}.$$  \hspace{1cm} (23)

It follows that the moment matrix $M$ has the following statistical bias.

$$E[\Delta M] = \sum_{\alpha=1}^{N} E[\Delta X_{\alpha}^\top W_{\alpha} \Delta X_{\alpha}]$$

$$= \sum_{\alpha=1}^{N} E\left[ \left( \Delta r'_{\alpha} - \Delta r_{\alpha}, W_{\alpha}(\Delta r'_{\alpha} - \Delta r_{\alpha}) \right) \right. $$

$$\left. - (\Delta r'_{\alpha} + \Delta r_{\alpha}) \times W_{\alpha}(\Delta r'_{\alpha} - \Delta r_{\alpha}) \right] \times W_{\alpha}(\Delta r'_{\alpha} + \Delta r_{\alpha}) \right)^T \right]\right],$$

Define a matrix $N$ as follows:

$$N = \begin{pmatrix} \frac{n}{N} n^\top & n \end{pmatrix},$$

$$n = \sum_{\alpha=1}^{N} (W_{\alpha}; V_0[r_{\alpha}]) + V_0[r'_{\alpha}],$$

$$n = -2 \sum_{\alpha=1}^{N} b_3[AW_{\alpha}(V_0[r_{\alpha}] - V_0[r'_{\alpha}])],$$

$$n' = \sum_{\alpha=1}^{N} (W_{\alpha} \times (V_0[r_{\alpha}] + V_0[r'_{\alpha}]).$$

The inner product $(A; B)$ of matrices $A = (A_{ij})$ and $B = (B_{ij})$ is defined by $(A; B) = \sum_{i,j=1}^{3} A_{ij}B_{ij}$. The exterior product $[A \times B]$ is the matrix whose $(i, j)$ element is $\sum_{k,l,m,n=1}^{3} \epsilon_{ijk}l \epsilon_{jmn}A_{km}B_{ln}$. The operation $A[.]$ designates antisymmetrization: $A[A] = (A - A^\top)/2$. For an antisymmetric matrix $C = (C_{ij})$, we define $t_3|C| = (C_{23}, C_{13}, C_{31})^T$. Then, the bias $E[\Delta M]$ is expressed as follows:

$$E[\Delta M] = \epsilon^2 N.$$  \hspace{1cm} (29)

Applying the recipe of Kanatani [10], we obtain the following renormalization procedure:

1. From the data $\{r_{\alpha}\}$ and $\{r'_{\alpha}\}$, compute $X_{\alpha}, \alpha = 1, \ldots, N$, by Eq. (16).
2. Set $c = 0$ and $W_{\alpha} = I$, $\alpha = 1, \ldots, N$.
3. Compute the moment matrix $M$ by Eq. (20).
4. Compute the matrix $N$ by Eq. (25).
5. Compute the smallest eigenvalue $\lambda$ of matrix $\hat{M} = M - cN$

$$\lambda$$

and the corresponding unit eigenvector $q = (q_0, q_1, q_2, q_3)^T$.
6. If $|\lambda| \approx 0$, return $q$ and stop. Otherwise, update $c$

$$C = C + \frac{\lambda}{|\lambda|^2}.$$  \hspace{1cm} (30)

5. Experiments

We conducted experiments for 3-D data obtained by stereo vision. Figures 1(a) and (b) are pairs of stereo images of an object before and after a rigid rotation around a vertical axis. We manually selected the feature points marked by black dots and computed their 3-D positions $r_{\alpha}$ and normalized covariance matrices $V_0[r_{\alpha}]$ by the method described in [11], assuming that image noise was isotropic and homogeneous (but the resulting errors in the reconstructed 3-D positions were highly anisotropic and inhomogeneous). We thus obtained two sets of 3-D points.

After translating one set so that its centroid coincides with that of the other, we computed the rotation by renormalization. In our experiment, we used $|\lambda| < 10^{-8}$ as the convergence criterion; we have confirmed that the result is not affected if it is in the range...
Table 1  Estimated rotations.

<table>
<thead>
<tr>
<th>Renormalization</th>
<th>Axis</th>
<th>Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(0.9999, 0.0003, 0.0123)</td>
<td>29.796°</td>
</tr>
<tr>
<td>Least squares</td>
<td>(0.9985, -0.0545, 0.0040)</td>
<td>26.790°</td>
</tr>
<tr>
<td>True values</td>
<td>(1.0000, 0.0000, 0.0000)</td>
<td>30.000°</td>
</tr>
</tbody>
</table>

(a) Renormalization.  (b) Least squares.

Fig. 2  Error distribution.

$10^{-10} \sim 10^{-5}$. As a comparison, we also tried the conventional least-squares method (the schemes described in [1], [5], [6], [9], [15]-[17] all yield the same solution). Table 1 lists the computed values together with the true values. We can see from this that our method considerably improves accuracy as compared with the least-squares method. However, this is for just one instance. In order to assert the superiority of our method, we need to examine the reliability of the solution for all possible occurrences of noise.

We evaluated the reliability of the computed solution $\hat{R}$ by applying a procedure called (parametric) bootstrap [3]. In the present case, we do not know the true positions $\{\hat{r}_n\}$, but we know the true rotation $R$ (see Table 1). So, we first estimate $\{\hat{\hat{\hat{r}}}_n\}$ by optimally correcting the data $\{r_n\}$ and $\{\hat{r}_n\}$ into $\{\hat{r}_n\}$ and $\{\hat{\hat{\hat{r}}}n\}$, respectively, so that the constraint $\hat{\hat{\hat{r}}}n = \hat{R}\hat{r}_n$ is exactly satisfied. This optimal correction is done as follows [10]:

$$\hat{r}_n = r_n + V_0[r_n] \hat{R}^\top \hat{W}_n(\hat{\hat{\hat{r}}}n - \hat{R}r_n),$$

$$\hat{W}_n = \left(\hat{R}V_0[r_n] \hat{R}^\top + V_0[r_n]\right)^{-1}.$$  

(33)  (34)

Estimating the variance $\epsilon^2$ by Eq. (12), we generated random independent Gaussian noise that has the estimated variance $\epsilon^2$ and added it to the projections of the corrected positions $\{\hat{\hat{\hat{r}}}_n\}$ and $\{\hat{\hat{\hat{r}}}'_n\}$ ($= \{\hat{\hat{\hat{r}}}_{\hat{\hat{\hat{r}}}}\}$) on the image planes of the left and the right cameras independently. Then, we computed the rotation $\hat{R}'$ and the error vector $\Delta\Omega'$ in the form given by Eq. (6).

Figure 2(a) shows three-dimensional plots of the error vector $\Delta\Omega'$ for 100 trials. The ellipsoid in the figure is defined by

$$(\Delta\Omega', \hat{V}[\hat{R}]^{-1}\Delta\Omega') = 1,$$

(35)

1If the true value $R$ is not known, its estimate $\hat{R}$ is used.

where $\hat{V}[\hat{R}]$ is the covariance matrix computed by approximating $\hat{R}$, $\{\hat{r}_n\}$, and $\epsilon^2$ by $\hat{R}$, $\{\hat{r}_n\}$, and $\epsilon^2$, respectively, on the right-hand side of eq. (8). This ellipsoid indicates the standard deviation of the errors in each orientation [10]; the cube in the figure is displayed as a reference. Figure 2(b) is the corresponding figure for the least-squares method (the ellipsoid and the cube are the same as in Fig. 2(a)).

Comparing Figs. 2(a) and (b), we can confirm that our method improves the accuracy of the solution considerably as compared with the least-squares method. We can also see that errors for our method distribute around the ellipsoid defined by Eq. (35), indicating that our method already attains the theoretical accuracy bound; no further improvement is possible.

The above visual observation can be given quantitative measures. We define the bootstrap mean $m_{\hat{R}}^*$ and the bootstrap covariance matrix $\hat{V}[\hat{R}]$ by

$$m_{\hat{R}}^* = \frac{1}{B} \sum_{b=1}^{B} \Delta \Omega_b,$$

$$\hat{V}[\hat{R}] = \frac{1}{B} \sum_{b=1}^{B} (\Delta \Omega_b^* - m_{\hat{R}}^*)(\Delta \Omega_b^* - m_{\hat{R}}^*)^\top,$$

(36)  (37)

where $B$ is the number of bootstrap samples and $\Delta \Omega_b^*$ is the error vector for the $b$th sample. The bootstrap mean error $E_{\hat{R}}$ and the bootstrap standard deviation $S_{\hat{R}}$ are defined by

$$E_{\hat{R}} = \|m_{\hat{R}}^*\|,$$

$$S_{\hat{R}} = \sqrt{\text{tr} \hat{V}[\hat{R}]}.$$

(38)

where $\text{tr} A$ denotes the trace of matrix $A$. The corresponding standard deviation for the (estimated) theoretical lower bound $\hat{V}[\hat{R}]$ is $\sqrt{\text{tr} \hat{V}[\hat{R}]}$. Table 2 lists the values of $E_{\hat{R}}$ and $S_{\hat{R}}$ for our method and the least-squares method ($B = 2000$) together with their theoretical lower bounds. We see from this that although the mean errors are very small for both methods, the standard deviation of our solution is almost 1/3 that of the least-squares solution and very close to the theoretical lower bound. The difference is due to statistical fluctuations; it also depends on the random numbers used for evaluation.

Thus, we can confirm that the reliability of the solution computed by our method can indeed be evaluated by (approximately) evaluating the theoretical accuracy bound given by Eq. (8).
6. Concluding Remarks

We have discussed optimal rotation estimation from two sets of 3-D points in the presence of anisotropic and inhomogeneous noise. We have first presented a theoretical accuracy bound defined independently of solution techniques and then given a method that attains it; our method is truly “optimal” in that sense. This optimal method is highly nonlinear, but we have shown that an efficient computational scheme can be obtained by using quaternions and applying the renormalization technique.

Since the solution attains the accuracy bound, we can view it as describing the reliability of the solution; the computation does not require any knowledge about the noise magnitude. Using real stereo images for 3-D reconstruction, we have demonstrated that our method is considerably more accurate than the conventional least-squares method. We have also confirmed the theoretical predictions of our theory by applying bootstrap procedure.

References


Naoya Ohta received his ME from the Tokyo Institute of Technology in 1985 and his Ph.D. from the University of Tokyo in 1998. He engaged in research and development of image processing systems at the Pattern Recognition Research Laboratory of NEC. He is currently Assistant Professor of computer science at Gunma University. He was a research affiliate of the Media Laboratory in MIT from 1991 to 1992.

Kenichi Kanatani received his Ph.D. in applied mathematics from the University of Tokyo in 1979. He is currently Professor of computer science at Gunma University. He is the author of Group-Theoretical Methods in Image Understanding (Springer, 1990), Geometric Computation for Machine Vision (Oxford University Press, 1993) and Statistical Optimization for Geometric Computation (Elsevier, 1996).