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A LEAST-SQUARES ALGORITHM FOR THE EQUIFORM TRANSFORMATION FROM SPATIAL MARKER CO-ORDINATES

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Abstract—The present paper describes an algorithm for estimating the translation vector and the rotation matrix of a moving body from noisy measurements on the spatial co-ordinates of at least three non-collinear markers. A sensitivity analysis of the estimated parameters and of the helical axis is presented in terms of characteristics of the marker distribution. The implementation of the proposed algorithm in a FORTRAN-subroutine is appended.

INTRODUCTION

An important aspect of the research on the kinematics of (parts of) the skeletal system is the determination of the motion of individual bones or body segments from measured data. It is assumed that the measured data are the co-ordinates in a fixed co-ordinate system of points, the so-called markers, at a number of points of time. These co-ordinates can be determined by X-ray stereo-photogrammetry or by any other suitable technique (Selvik, 1974; Woltring, 1982).

In this paper only the motion of one bone from time t_1 to time t_2 is considered. If the bone is assumed to be rigid, many algorithms are available to determine the kinematical parameters (translation vector, rotation matrix, helical axis etc.) that characterize the motion from time t_1 to time t_2 (Rodrigues, 1840; Kinzel *et al.*, 1972; Selvik, 1974; Chao, 1978; Panjabi and White, 1971; Youm and Yoon, 1979; Spoor and Veldpaus, 1980 etc.). The method to be discussed in this paper comes close to the method given by Spoor and Veldpaus (1980). An unweighted least-squares method is employed to determine the primary unknowns, being a translation vector \mathbf{r} and the rotation matrix \mathbf{R} of the bone at time t_2 with respect to time t_1 . All other kinematical parameters, like the helical axis, are secondary unknowns that can be estimated as soon as \mathbf{r} and \mathbf{R} are known.

Some of the disadvantages of the algorithm of Spoor and Veldpaus (1980), especially the calculation of the eigenvectors of a 3×3 matrix, are avoided here. Furthermore, the formulation in this paper is more suitable for analyzing the sensitivity of the kinematical parameters to small disturbances in the measured co-ordinates of the markers.

SOME GENERAL REMARKS

Let P_1, P_2, \dots, P_m ($m \geq 3$) be the markers, attached to the body (e.g. a bone) under consideration. The position vector of P_i (strictly: the column matrix containing the co-ordinates of P_i with respect to a fixed, orthogonal co-ordinate system) at time $t = t_1$ is denoted by \mathbf{a}_i . An important characteristic of the marker distribution is the position vector \mathbf{a} of the centre P_0 of that distribution at time $t = t_1$:

$$\mathbf{a} = \frac{1}{m} \sum_{i=1}^m \mathbf{a}_i. \quad (2.1)$$

Another characteristic is the distribution matrix A which only depends on the relative position vectors $\mathbf{a}_i - \mathbf{a}$ of the P_i ($i = 1, 2, \dots, m$) with respect to the centre P_0 . This matrix is given by

$$A = \frac{1}{m} \sum_{i=1}^m (\mathbf{a}_i - \mathbf{a})(\mathbf{a}_i - \mathbf{a})^T \quad (2.2)$$

where the superscript T denotes transposition. From this definition it is seen that A is symmetric and semi-positive definite (Gantmacher, 1977). As a consequence, the eigenvalues α_1, α_2 and α_3 of A are real, non-negative numbers, which can be ordered such that $\alpha_1 \geq \alpha_2 \geq \alpha_3 \geq 0$. Without any restriction the corresponding unit eigenvectors $\boldsymbol{\eta}_1, \boldsymbol{\eta}_2$ and $\boldsymbol{\eta}_3$ may be assumed to be mutually orthogonal, i.e. $\boldsymbol{\eta}_j^T \boldsymbol{\eta}_k = \delta_{jk}$ for $j, k = 1, 2, 3$. Here, δ_{jk} is the Kronecker-delta ($\delta_{jk} = 1$ if $j = k$ and $\delta_{jk} = 0$ otherwise). As a result, A is given (in spectral representation) by:

$$A = \sum_{j=1}^3 \alpha_j \boldsymbol{\eta}_j \boldsymbol{\eta}_j^T; \boldsymbol{\eta}_j^T \boldsymbol{\eta}_k = \delta_{jk} \quad \text{for } j, k = 1, 2, 3. \quad (2.3)$$

A marker distribution is 3-dimensional or spatial if all eigenvalues of A differ significantly from zero. Then A is a regular matrix with positive determinant, i.e. $\det(A) = \alpha_1 \alpha_2 \alpha_3 > 0$. In this case the rank of A .

denoted by $rk(A)$, is equal to 3. A marker distribution is 2-dimensional or planar if the smallest eigenvalue of A , α_3 , is equal to zero while the other eigenvalues, α_1 and α_2 , differ significantly from zero and are of the same order of magnitude. In this case A is singular: $\det(A) = 0$ and $rk(A) = 2$. If only one eigenvalue of A differs significantly from zero, i.e. if $\alpha_1 > 0$ and $\alpha_2 = \alpha_3 = 0$, the marker distribution is 1-dimensional or linear. Then $\det(A) = 0$ and $rk(A) = 1$. In the sequel it is assumed that the marker distribution is spatial or at least planar, which implies that $rk(A) \geq 2$. Apart from the mean position vector \mathbf{a} the matrix A will appear to be the only relevant characteristic of the marker distribution.

If the body is rigid, the motion from time $t = t_1$ to time $t = t_2$ can be described in terms of the sum of the translation of P_0 , characterized by the translation vector \mathbf{r} , and a rotation around P_0 , characterized by the rotation matrix R which of course satisfies

$$R^T R = I; \quad \det(R) = +1. \quad (2.4)$$

In this case, the position vector \mathbf{p}_i of P_i ($i = 1, 2, \dots, m$) at time $t = t_2$ is related to the position vector \mathbf{a}_i of P_i at time $t = t_1$ by the isometric (or Euclidean) transformation

$$\mathbf{p}_i = \mathbf{a} + \mathbf{r} + R(\mathbf{a}_i - \mathbf{a}). \quad (2.5)$$

For simplicity, in the remainder of this paper the position vectors $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_m$ of the markers at time $t = t_1$ are considered error-free. If necessary, errors in these vectors can be taken into account with slight modifications of the equations. Due to the fact that a real body is not perfectly rigid and due to measurement errors the measured position vectors $\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2, \dots, \hat{\mathbf{p}}_m$ of the markers at time $t = t_2$ will differ from the exact values $\mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_m$ at that time. As a consequence, it is impossible to determine the exact translation vector \mathbf{r} and the exact rotation matrix R from measured data.

THE UNWEIGHTED LEAST-SQUARES PROCEDURE

To determine an approximation $\hat{\mathbf{r}}$ for the exact translation vector \mathbf{r} of the centre P_0 of the marker distribution and an approximation \hat{H} for the exact rotation matrix R a least squares method is used, where markers are treated with the same weight. It is assumed that the best approximations for \mathbf{r} and R are the vector $\hat{\mathbf{r}}$ and the matrix \hat{H} that minimize the least-squares function $f = f(\mathbf{r}, H)$, defined by:

$$f(\hat{\mathbf{r}}, \hat{H}) = \frac{1}{m} \sum_{i=1}^m [(\hat{\mathbf{p}}_i - \mathbf{a} - \hat{\mathbf{r}} - \hat{H}(\mathbf{a}_i - \mathbf{a}))^T \times (\hat{\mathbf{p}}_i - \mathbf{a} - \hat{\mathbf{r}} - \hat{H}(\mathbf{a}_i - \mathbf{a}))]. \quad (3.1)$$

Here, the vector $\hat{\mathbf{p}}_i - \mathbf{a} - \hat{\mathbf{r}} - \hat{H}(\mathbf{a}_i - \mathbf{a})$ is the difference between the measured vector $\hat{\mathbf{p}}_i$ of P_i ($i = 1, 2, \dots, m$) at time $t = t_2$ and the fitted vector $\mathbf{a} + \hat{\mathbf{r}} + \hat{H}(\mathbf{a}_i - \mathbf{a})$ of P_i at that time. Requiring $f = f(\hat{\mathbf{r}}, \hat{H})$ to be minimal means that the fitted positions of the markers must be as close as possible to the measured positions. It can

easily be shown from the definition that $f = f(\hat{\mathbf{r}}, \hat{H})$ is given by:

$$f(\hat{\mathbf{r}}, \hat{H}) = (\hat{\mathbf{p}} - \mathbf{a} - \hat{\mathbf{r}})^T (\hat{\mathbf{p}} - \mathbf{a} - \hat{\mathbf{r}}) + \text{tr}(\hat{P} - 2\hat{G}\hat{H}^T + \hat{H}A\hat{H}^T) \quad (3.2)$$

where the trace of a matrix D (i.e. the sum of the diagonal components of D) is denoted by $\text{tr}(D)$ and the vector $\hat{\mathbf{p}}$ and the matrices \hat{P} and \hat{G} are defined by:

$$\hat{\mathbf{p}} = \frac{1}{m} \sum_{i=1}^m \hat{\mathbf{p}}_i \quad (3.3)$$

$$\hat{G} = \frac{1}{m} \sum_{i=1}^m ((\hat{\mathbf{p}}_i - \hat{\mathbf{p}})(\mathbf{a}_i - \mathbf{a})^T) \quad (3.4)$$

$$\hat{P} = \frac{1}{m} \sum_{i=1}^m ((\hat{\mathbf{p}}_i - \hat{\mathbf{p}})(\hat{\mathbf{p}}_i - \hat{\mathbf{p}})^T). \quad (3.5)$$

Hence, $\hat{\mathbf{p}}$ may be considered as the position vector of the centre of the measured marker distribution at time $t = t_2$. Furthermore, it is seen that \hat{P} plays a similar role for the measured distribution at time $t = t_2$ as A for the distribution at time $t = t_1$. In \hat{G} both the measured relative position vectors at time $t = t_2$ and the relative position vectors at time $t = t_1$ appear.

It is not necessary to require *a priori* that \hat{H} is a rotation matrix. If no constraint conditions are imposed on \hat{H} the minimum of $f = f(\hat{\mathbf{r}}, \hat{H})$ can be found by requiring that for each infinitesimal small variation $\delta\mathbf{r}$ of $\hat{\mathbf{r}}$ and δH of \hat{H} the first variation $\delta f = f(\hat{\mathbf{r}} + \delta\mathbf{r}, \hat{H} + \delta H) - f(\hat{\mathbf{r}}, \hat{H})$ of $f = f(\hat{\mathbf{r}}, \hat{H})$ must be zero. For variations of $\hat{\mathbf{r}}(\delta\mathbf{r} \neq 0$ and $\delta H = 0)$ this requirement yields:

$$\hat{\mathbf{r}} = \hat{\mathbf{p}} - \mathbf{a} \quad (3.6)$$

while variations of \hat{H} ($\delta\mathbf{r} = 0$ and $\delta H \neq 0$) result in $\text{tr}(-2\hat{G}\delta H^T + \delta H A \hat{H}^T + \hat{H} A \delta H^T) = 0$ for each δH^T (3.7)

and because $\text{tr}(\delta H A \hat{H}^T) = \text{tr}(\hat{H} A \delta H^T)$ this is satisfied only if

$$\hat{H} A = \hat{G}. \quad (3.8)$$

In the ideal case, i.e. in the absence of any deformation of the body and of measurement errors, the vectors $\hat{\mathbf{p}}_i$ ($i = 1, 2, \dots, m$) coincide with the exact vectors $\mathbf{p}_i = \mathbf{a} + \mathbf{r} + R(\mathbf{a}_i - \mathbf{a})$. Hence, $\hat{\mathbf{p}} = \mathbf{a} + \mathbf{r}$ and $\hat{G} = R A$, which implies that $\hat{\mathbf{r}} = \mathbf{r}$ and $\hat{H} = R$. Therefore, the least squares procedure yields the exact results for $\hat{\mathbf{r}}$ and \hat{H} in the ideal case. In practise, however the matrix \hat{H} as determined from (3.8) is not a rotation matrix, i.e. $\hat{H}^T \hat{H} \neq I$. Therefore, an additional calculation is necessary to extract from \hat{H} the information about the rotation of the body. Such a calculation can be based on the polar decomposition theorem (Chadwick, 1976), which states that the 3×3 matrix \hat{H} can be written as the product of a 3×3 rotation matrix \hat{R} and a symmetrical 3×3 matrix \hat{U} :

$$\hat{H} = \hat{R} \hat{U}; \quad \hat{U} = \hat{U}^T; \quad \hat{R}^T \hat{R} = I; \quad \det(\hat{R}) = +1. \quad (3.9)$$

The matrix $\hat{U} - I$ represents a homogeneous deformation of the body (Chadwick, 1976). For a rigid body \hat{U} should be equal to I . In general this will not be the case. The difference $\hat{U} - I$ gives some information about the accuracy of the measured data and about the validity of the assumption that the body is rigid. However, it is impossible to distinguish between the contribution of measurement errors and the contribution of a possible deformation of the body. Besides, it can be proven that a spatial distribution of markers (i.e. $m \geq 4$) is required for a unique determination of \hat{U} . An interesting potentiality of this version of the least-squares method is the use of it to quantify homogeneous size changes of the body, for instance due to growth. Nevertheless, this version is not considered anymore in this paper and constraints are imposed on \hat{H} .

Usually it is required that \hat{H} is a rotation matrix. Writing \hat{R} instead of \hat{H} to emphasize this, the least-squares method leads to determination of \hat{f} and \hat{R} such that the function $f = f(\hat{f}, \hat{R})$, defined by

$$f(\hat{f}, \hat{R}) = (\hat{p} - \mathbf{a} - \hat{f})^T (\hat{p} - \mathbf{a} - \hat{f}) + \text{tr}(\hat{P} - 2\hat{G}\hat{R}^T + \hat{R}\hat{A}\hat{R}^T), \quad (3.10)$$

is minimized under the constraint conditions

$$\hat{R}^T \hat{R} = I; \quad \det(\hat{R}) = +1.$$

This formulation, used for instance by Spoor and Veldpaus (1980), has the disadvantage that the results, \hat{f} and \hat{R} contain no information at all to check the assumed rigidity of the body. An advantage is that only three non-collinear markers are required for uniqueness of \hat{R} . To maintain this advantage and to avoid more or less the mentioned disadvantage it is assumed in this paper that \hat{H} is a matrix of the form $\hat{s}\hat{R}$ with a positive scalar \hat{s} and a rotation matrix \hat{R} . The least-squares method then results in the problem to determine \hat{s} , \hat{f} and \hat{R} such that the function $f = f(\hat{s}, \hat{f}, \hat{R})$ defined by

$$f(\hat{s}, \hat{f}, \hat{R}) = (\hat{p} - \mathbf{a} - \hat{f})^T (\hat{p} - \mathbf{a} - \hat{f}) + \text{tr}(\hat{P} - 2\hat{s}\hat{G}\hat{R}^T + \hat{s}^2\hat{R}\hat{A}\hat{R}^T) \quad (3.11)$$

is minimized under the constraint conditions

$$\hat{s} > 0; \quad \hat{R}^T \hat{R} = I; \quad \det(\hat{R}) = +1. \quad (3.12)$$

The value of \hat{s} will give some information about the quality of the measurement: if \hat{s} differs from the exact value 1 the body does not behave as a rigid body and/or the measured data are inaccurate.

Several methods are known to take some or all constraint conditions into account. A commonly used method with respect to the condition $\hat{R}^T \hat{R} = I$ is based on the observation that this symmetrical matrix equation constitutes a set of six independent scalar equations in the nine components of \hat{R} . Hence, these components can be written as a function of three independent scalar quantities $\hat{\phi}_1$, $\hat{\phi}_2$ and $\hat{\phi}_3$, for instance Euler or Cardan angles (Wittenburg, 1977).

These quantities are the components of a column $\hat{\phi}$ and \hat{R} can be seen as a function of $\hat{\phi}$ i.e. $\hat{R} = R(\hat{\phi})$, such that $R^T(\phi)R(\phi) = I$ and $\det(R(\phi)) = +1$ for each ϕ . The least-squares function then becomes a function of \hat{s} , \hat{f} and $\hat{\phi}$ and this function must be minimized under the remaining constraint condition $\hat{s} > 0$. The most important drawbacks of this method are that the elaboration is quite digressive, that sometimes special precautions have to be taken to arrive at a solution for $\hat{\phi}$ and that the elaboration must be done again if another choice for $\hat{\phi}_1$, $\hat{\phi}_2$ and $\hat{\phi}_3$ (for instance, Cardan angles instead of Euler angles) is wanted. For these reasons another method is used by taking the constraint equation $\hat{R}^T \hat{R} = I$ into account with the Lagrange multiplier theorem. For this purpose a term $\text{tr}(I - \hat{R}^T \hat{R})L$ is added to the original least squares function $f = f(\hat{s}, \hat{f}, \hat{R})$, where L is a matrix with as yet unknown Lagrange multipliers. This yields the modified least-squares function $F = F(\hat{s}, \hat{f}, \hat{R}, L)$:

$$F(\hat{s}, \hat{f}, \hat{R}, L) = f(\hat{s}, \hat{f}, \hat{R}) - \text{tr}((\hat{R}^T \hat{R} - I)L). \quad (3.13)$$

Let \hat{s} , \hat{f} , \hat{R} and L result in a stationary value of this modified function. The Lagrange multiplier theorem then states that \hat{s} , \hat{f} and \hat{R} also result in a stationary (not necessarily a minimal!) value of the original function. In this way the constraint conditions $\hat{s} > 0$ and $\det(\hat{R}) = +1$ are not taken into account and it must be verified *a posteriori* whether these conditions are satisfied for the determined values of \hat{s} , \hat{f} and \hat{R} and whether these values result in a minimum of the original function.

Stationary values of $F = F(\hat{s}, \hat{f}, \hat{R}, L)$ are obtained if the first variation δF of F is zero for each infinitesimal small variation of \hat{s} , \hat{f} , \hat{R} and L . It is shown in Appendix A that this results in the following set of equations:

$$\hat{f} = \hat{p} - \mathbf{a} \quad (3.14)$$

$$\hat{s} \text{tr}(\hat{A}) = \text{tr}(\hat{B}) \quad (3.15)$$

$$\hat{R}^T \hat{R} = I; \quad \hat{G} = \hat{R} \hat{B} \quad (3.16)$$

where \hat{B} is a symmetrical matrix, defined by:

$$\hat{B} = \hat{s}\hat{A} - \frac{1}{2\hat{s}}(L + L^T). \quad (3.17)$$

A solution of these equations is the solution of the original problem if and only if $\hat{s} > 0$, $\det(\hat{R}) = +1$ and $f(\hat{s}, \hat{f}, \hat{R})$ is minimal. From $\hat{s} > 0$ and $\text{tr}(\hat{A}) = \alpha_1 + \alpha_2 + \alpha_3 > 0$ it follows from (3.15) that $\text{tr}(\hat{B})$ must be positive. Besides it is seen from $\det(\hat{R}) = +1$ and $\hat{G} = \hat{R} \hat{B}$ that $\det(\hat{B})$ must be equal to $\det(\hat{G})$. Finally, it is shown in Appendix A that the value of the original least-squares function at a stationary point is equal to $\text{tr}(\hat{P}) - \hat{s} \text{tr}(\hat{B})$. Because $\text{tr}(\hat{P})$ is a positive number, completely determined by the measured data, $\text{tr}(\hat{P}) - \hat{s} \text{tr}(\hat{B})$ represents a minimum of the original function if $\text{tr}(\hat{B})$ is maximal. Hence, the solution for \hat{s} , \hat{f} and \hat{R} of the original problem satisfies (3.14), (3.15) and

(3.16) and the additional requirements

$$\text{tr}(\hat{B}) > 0; \text{tr}(\hat{B}) \text{ maximal}; \det(\hat{B}) = \det(\hat{G}). \quad (3.18)$$

DETERMINATION OF THE ROTATION MATRIX

The starting point for the determination of \hat{R} is given by (3.16). The decomposition of \hat{G} in the product of \hat{R} and \hat{B} is the earlier mentioned polar decomposition of \hat{G} (Tienstra (1969), Chadwick (1976), Stephenson (1980)). Using $\hat{R}^T \hat{R} = I$ and $\hat{B} = \hat{B}^T$ it follows that

$$\hat{G}^T \hat{G} = \hat{B}^T \hat{B} = \hat{B}^2. \quad (4.1)$$

Because $\hat{G}^T \hat{G}$ is symmetrical and semi-positive definite, the eigenvalues of $\hat{G}^T \hat{G}$ are real and non-negative. Let $\hat{\mu}_1, \hat{\mu}_2$, and $\hat{\mu}_3$ be non-negative numbers, such that $\hat{\mu}_1 \geq \hat{\mu}_2 \geq \hat{\mu}_3 \geq 0$ and that $\hat{\mu}_1^2, \hat{\mu}_2^2$ and $\hat{\mu}_3^2$ are the eigenvalues of $\hat{G}^T \hat{G}$. Let \hat{n}_1, \hat{n}_2 and \hat{n}_3 be the corresponding, mutually orthogonal unit eigenvectors of $\hat{G}^T \hat{G}$. Then the spectral representation of this matrix is given by:

$$\hat{G}^T \hat{G} = \sum_{j=1}^3 (\hat{\mu}_j^2 \hat{n}_j \hat{n}_j^T); \hat{n}_j^T \hat{n}_k = \delta_{jk} \text{ for } j, k = 1, 2, 3. \quad (4.2)$$

The matrix \hat{B} is symmetrical too. Let $\hat{\lambda}_1, \hat{\lambda}_2$ and $\hat{\lambda}_3$ be the eigenvalues of \hat{B} and let $\mathbf{n}_1^*, \mathbf{n}_2^*$ and \mathbf{n}_3^* be the corresponding, mutually orthogonal unit eigenvectors of \hat{B} . From (4.1) it follows that the eigenvectors of \hat{B} must coincide with the eigenvectors of $\hat{G}^T \hat{G}$ and that the squared eigenvalues of \hat{B} must be equal to the eigenvalues of $\hat{G}^T \hat{G}$, i.e. $\mathbf{n}_j^* = \hat{n}_j$ and $\hat{\lambda}_j^2 = \hat{\mu}_j^2$ for $j = 1, 2, 3$. For \hat{B} this results in:

$$\hat{B} = \sum_{j=1}^3 (\hat{\lambda}_j \hat{n}_j \hat{n}_j^T); \hat{\lambda}_j = \tau_j \hat{\mu}_j; \tau_j^2 = 1 \text{ for } j = 1, 2, 3. \quad (4.3)$$

The signs τ_1, τ_2 and τ_3 follow from the additional requirements (3.18). From $\det(\hat{B}) = \det(\hat{G})$ and $\det(\hat{B}) = \hat{\lambda}_1 \hat{\lambda}_2 \hat{\lambda}_3$ it is seen that τ_1, τ_2 and τ_3 have to satisfy

$$\tau_1 \tau_2 \tau_3 = \tau; \quad \tau = \text{sign}(\det(\hat{G})). \quad (4.4)$$

Furthermore, $\text{tr}(\hat{B})$ must be positive and therefore $\tau_1 \hat{\mu}_1 + \tau_2 \hat{\mu}_2 + \tau_3 \hat{\mu}_3 > 0$. Finally, $\text{tr}(\hat{B})$ must be maximal and because $\hat{\mu}_1 \geq \hat{\mu}_2 \geq \hat{\mu}_3 \geq 0$ this will be the case if $\tau_1 = \tau_2 = +1$ and $\tau_3 = \tau$, i.e.

$$\hat{\lambda}_1 = \hat{\mu}_1; \quad \hat{\lambda}_2 = \hat{\mu}_2; \quad \hat{\lambda}_3 = \tau \hat{\mu}_3. \quad (4.5)$$

For a given matrix \hat{G} the sign τ of $\det(\hat{G})$, the eigenvalues $\hat{\mu}_1^2, \hat{\mu}_2^2$ and $\hat{\mu}_3^2$ and the eigenvectors \hat{n}_1, \hat{n}_2 and \hat{n}_3 can be calculated. Then \hat{B} follows from (4.3) and (4.5) and \hat{R} must be determined from $\hat{G} = \hat{R} \hat{B}$. This (more or less conventional) approach was followed by Spoor and Veldpaus (1980). However, \hat{B} itself is of no interest and it will be shown that \hat{R} can be calculated in a more direct way without explicit determination of \hat{B} . This alternative approach is based on the

Cayley–Hamilton theorem (Gantmacher, 1977), which states that each matrix satisfies its own characteristic equation. For \hat{B} this yields:

$$\hat{B}^2 - \hat{\beta}_1 \hat{B} + \hat{\beta}_2 I = \hat{B}^a \quad (4.6)$$

where $\hat{\beta}_1$ and $\hat{\beta}_2$ are the first and the second invariants of \hat{B} :

$$\hat{\beta}_1 = \text{tr}(\hat{B}) = \hat{\lambda}_1 + \hat{\lambda}_2 + \hat{\lambda}_3 = \hat{\mu}_1 + \hat{\mu}_2 + \tau \hat{\mu}_3 \quad (4.7)$$

$$\begin{aligned} \hat{\beta}_2 &= \text{tr}(\hat{B}^a) = \hat{\lambda}_1 \hat{\lambda}_2 + \hat{\lambda}_2 \hat{\lambda}_3 + \hat{\lambda}_3 \hat{\lambda}_1 \\ &= \hat{\mu}_1 \hat{\mu}_2 + \tau \hat{\mu}_3 (\hat{\mu}_1 + \hat{\mu}_2). \end{aligned} \quad (4.8)$$

The matrix \hat{B}^a is the so-called adjoint of \hat{B} . A definition and some properties of adjoint matrices are given in Appendix B. From this Appendix and from $\hat{B} = \hat{R}^T \hat{G}$ it is seen that $\hat{B}^a = \hat{R}^T \hat{G}^a$. Using this result in (4.6) and replacing \hat{B} and \hat{B}^2 by $\hat{R}^T \hat{G}$ and $\hat{G}^T \hat{G}$, respectively, results in:

$$\hat{R} \hat{C} = \hat{G}^a + \hat{\beta}_1 \hat{G}; \quad \hat{C} = \hat{G}^T \hat{G} + \hat{\beta}_2 I. \quad (4.9)$$

A further investigation of the matrix \hat{C} is given in the next section. Here it is assumed that \hat{C} is regular. Then \hat{R} follows from (4.9) as:

$$\hat{R} = (\hat{G}^a + \hat{\beta}_1 \hat{G}) \hat{C}^{-1}. \quad (4.10)$$

Hence, \hat{R} can be determined without explicit calculation of \hat{B} . Nevertheless, the invariants $\hat{\beta}_1$ and $\hat{\beta}_2$ must be known. They can be calculated by first determining the eigenvalues $\hat{\mu}_1^2, \hat{\mu}_2^2$ and $\hat{\mu}_3^2$ of $\hat{G}^T \hat{G}$ and then using the definitions (4.7) and (4.8). However, another method is possible. From (4.7) and (4.8) it is seen that

$$\hat{\beta}_1^2 - 2\hat{\beta}_2 = \hat{g}_1^2; \quad \hat{\beta}_2^2 = \hat{g}_2^2 + 2\hat{\beta}_1 \hat{g}_3 \quad (4.11)$$

where \hat{g}_1^2 and \hat{g}_2^2 are the first and second invariants of $\hat{G}^T \hat{G}$ while \hat{g}_3 is equal to the determinant of \hat{G} :

$$\hat{g}_1^2 = \text{tr}(\hat{G}^T \hat{G}) = \hat{\mu}_1^2 + \hat{\mu}_2^2 + \hat{\mu}_3^2 \quad (4.12)$$

$$\hat{g}_2^2 = \text{tr}(\hat{G}^T \hat{G})^2 = \hat{\mu}_1^2 \hat{\mu}_2^2 + \hat{\mu}_2^2 \hat{\mu}_3^2 + \hat{\mu}_3^2 \hat{\mu}_1^2 \quad (4.13)$$

$$\hat{g}_3 = \det(\hat{G}) = \tau \hat{\mu}_1 \hat{\mu}_2 \hat{\mu}_3. \quad (4.14)$$

The invariant $\hat{\beta}_2$ is positive for each acceptable set of measurements as will be shown in the next section. Besides, $\hat{\beta}_1$ is positive. This implies that $\hat{\beta}_1$ and $\hat{\beta}_2$ are determined uniquely by (4.11). These non-linear equations can be solved in an iterative way, for instance by means of the Newton–Raphson method. This is outlined in Appendix C. In Appendix E a subroutine, called POLDEC, is given. For a given matrix \hat{G} this subroutine first calculates the matrices \hat{G}^a and $\hat{G}^T \hat{G}$ and the scalars \hat{g}_1^2, \hat{g}_2^2 and \hat{g}_3 , then determines the invariants $\hat{\beta}_1$ and $\hat{\beta}_2$ in an iterative way and finally calculates the rotation matrix \hat{R} from (4.9) and (4.10). The calculated value for $\hat{\beta}_1$ can also be used to determine the factor \hat{s} from (3.15).

NUMERICAL STABILITY

From a numerical point of view the matrix \hat{C} is of

particular interest. Using (4.2) for $\hat{G}^T \hat{G}$ yields:

$$\hat{C} = \hat{G}^T \hat{G} + \hat{\beta}_2 I = \sum_{j=1}^3 (\hat{\gamma}_j \hat{\mathbf{n}}_j \hat{\mathbf{n}}_j^T); \quad \hat{\gamma}_j = \hat{\mu}_j^2 + \hat{\beta}_2$$

for $j = 1, 2, 3$ (5.1)

and with the definition (4.8) of $\hat{\beta}_2$ it follows that the eigenvalues of \hat{C} are equal to

$$\begin{aligned} \hat{\gamma}_1 &= (\hat{\mu}_1 + \tau \hat{\mu}_3)(\hat{\mu}_1 + \hat{\mu}_2); \\ \hat{\gamma}_2 &= (\hat{\mu}_2 + \hat{\mu}_1)(\hat{\mu}_2 + \tau \hat{\mu}_3) \\ \hat{\gamma}_3 &= (\tau \hat{\mu}_3 + \hat{\mu}_1)(\tau \hat{\mu}_3 + \hat{\mu}_2). \end{aligned} \quad (5.2)$$

From $\hat{\mu}_1 \geq \hat{\mu}_2 \geq \hat{\mu}_3 \geq 0$ and $\tau = \pm 1$ it can be seen that $\hat{\gamma}_1 \geq \hat{\gamma}_2 \geq \hat{\gamma}_3 \geq 0$. The determinant of \hat{C} is given by

$$\det(\hat{C}) = \hat{\gamma}_1 \hat{\gamma}_2 \hat{\gamma}_3 = \hat{v}^2; \quad \hat{v} = (\hat{\mu}_1 + \hat{\mu}_2)(\hat{\mu}_2 + \tau \hat{\mu}_3)(\tau \hat{\mu}_3 + \hat{\mu}_1). \quad (5.3)$$

Hence \hat{C} is regular, i.e. $\det(\hat{C}) \neq 0$, if $\hat{\mu}_3 > -\tau \hat{\mu}_2$. This implies that the determination of \hat{R} from (4.10) is possible if and only if $\hat{\mu}_3 > -\tau \hat{\mu}_2$. A measure for the numerical stability of the calculation of \hat{R} is given by the condition number $c(\hat{C})$ of the matrix \hat{C} . This number is equal to the quotient of the largest and smallest eigenvalue of \hat{C} , i.e.

$$c(\hat{C}) = \frac{\hat{\gamma}_1}{\hat{\gamma}_3} = \frac{\hat{\mu}_1 + \hat{\mu}_2}{\hat{\mu}_2 + \tau \hat{\mu}_3}. \quad (5.4)$$

Of course $1 \leq c(\hat{C})$. If $c(\hat{C})$ is very large ($c(\hat{C}) \gg 1$) the matrix \hat{C} is ill-conditioned and numerical problems can arise in the calculation of \hat{R} from (4.10).

To obtain more information about $c(\hat{C})$ the ideal case is considered first. Denoting the exact values of \hat{G} , \hat{R} , $\hat{\beta}$, etc. by G , R , β , etc. and using (2.3) it is easily shown that:

$$G = RA; \quad (5.5)$$

$$G^T G = A^2; \quad \mu_j = \alpha_j \quad \text{for } j = 1, 2, 3 \quad (5.6)$$

$$\beta_2 = \alpha_1 \alpha_2 + \alpha_2 \alpha_3 + \alpha_3 \alpha_1 > 0 \quad (5.7)$$

$$c(C) = \frac{\alpha_1 + \alpha_2}{\alpha_2 + \alpha_3}. \quad (5.8)$$

As stated before collinear distributions of markers are left out of consideration. For (nearly) planar marker distribution α_1 and α_2 differ significantly from zero and are of the same order of magnitude while α_3 is zero or very small. In this case $c(C)$ will not be smaller than but close to 2. For a spatial marker distribution α_1 , α_2 and α_3 differ significantly from zero and are of the same order of magnitude. This means that $c(C)$ will be not smaller than but close to 1.

Due to deformations and/or measurement errors \hat{G} will differ from G and, more importantly, $\hat{\mu}_1$, $\hat{\mu}_2$ and $\hat{\mu}_3$ will not be equal to the eigenvalues α_1 , α_2 and α_3 of A . A set of measurements will be called acceptable if the differences are small compared with the maximum eigenvalue α_1 , i.e. if

$$|\hat{\mu}_j - \alpha_j| \ll \alpha_1 \quad \text{for } j = 1, 2, 3. \quad (5.10)$$

In the sequel only acceptable measurements are considered. For a spatial distribution of markers this means that $\hat{\mu}_1$, $\hat{\mu}_2$ and $\hat{\mu}_3$ differ significantly from zero, that $\det(\hat{G}) > 0$ and hence $\tau = +1$. Then $c(\hat{C})$ is approximately equal to $c(C)$, \hat{C} is a well-conditioned matrix and no numerical problems are to be expected. Besides, β_2 will be positive. For a planar distribution $\hat{\mu}_1$ and $\hat{\mu}_2$ differ significantly from zero while $\hat{\mu}_3$ can differ from zero but will be small compared to both $\hat{\mu}_1$ and $\hat{\mu}_2$. Also in this case $c(\hat{C})$ will be approximately equal to $c(C)$ and \hat{C} will be well-conditioned. However, $\det(\hat{G})$ can be negative and hence $\tau = -1$. From the definition (4.8) of $\hat{\beta}_2$ it then follows $\hat{\beta}_2 = \hat{\mu}_1 \hat{\mu}_2 - \hat{\mu}_3(\hat{\mu}_1 + \hat{\mu}_2)$, so $\hat{\beta}_2 > 0$ if $\hat{\mu}_3 < 1/2 \hat{\mu}_2$. Recalling that, in the ideal case, $\mu_3 = \hat{\mu}_3 = 0$ for a planar distribution while $\hat{\mu}_2$ differs significantly from zero it is clear that $\hat{\beta}_2$ will be positive for any acceptable set of measurements.

SENSITIVITY ANALYSIS

The position vectors $\hat{\mathbf{p}}_1, \hat{\mathbf{p}}_2, \dots, \hat{\mathbf{p}}_m$ of the markers at time $t = t_2$ are subject to measurement errors. Some information about the influence of these errors on the final results $\hat{\mathbf{s}}$, $\hat{\mathbf{r}}$ and \hat{R} can be gained by disturbing the vectors $\hat{\mathbf{p}}_i$ ($i = 1, 2, \dots, m$) by small vectors $\Delta \mathbf{p}_i$. The associated disturbances $\Delta \mathbf{p}$ and ΔG of the mean vector $\hat{\mathbf{p}}$ and the matrix \hat{G} , respectively, are given by:

$$\Delta \mathbf{p} = \frac{1}{m} \sum_{i=1}^m \Delta \mathbf{p}_i; \quad \Delta G = \frac{1}{m} \sum_{i=1}^m ((\Delta \mathbf{p}_i - \Delta \mathbf{p})(\mathbf{a}_i - \mathbf{a})^T) \quad (6.1)$$

and from (3.14) it is seen that the disturbance $\Delta \mathbf{r}$ of the translation vector $\hat{\mathbf{r}}$ of the centre P_0 of the marker distribution is equal to $\Delta \mathbf{p}$:

$$\Delta \mathbf{r} = \Delta \mathbf{p}. \quad (6.2)$$

To derive an expression for the disturbance ΔR of \hat{R} it is noted that both \hat{R} and $\hat{R} + \Delta R$ are orthogonal, so

$$(\hat{R} + \Delta R)^T (\hat{R} + \Delta R) = I; \quad \hat{R}^T \hat{R} = I. \quad (6.3)$$

If the disturbances are small the term $\Delta R^T \Delta R$ in (6.3) may be neglected with respect to the other terms and (6.3) reduces to

$$\hat{R}^T \Delta R = -\Delta R^T \hat{R} = -(\hat{R}^T \Delta R)^T, \quad (6.4)$$

which states that $\hat{R}^T \Delta R$ is skew-symmetrical. Hence, there exists a vector $\Delta \mathbf{v}$, the so-called axial vector of $\hat{R}^T \Delta R$ (Chadwick (1976)), such that the following relation holds for each vector \mathbf{w} :

$$(R^T \Delta R) \mathbf{w} = \Delta \mathbf{v} * \mathbf{w}, \quad (6.5)$$

where $*$ denotes the vector product operator. If $\Delta \mathbf{v}$ and R are known the matrices $\hat{R}^T \Delta R$ and ΔR are determined uniquely and therefore it suffices to determine $\Delta \mathbf{v}$ instead of ΔR .

To relate $\Delta \mathbf{v}$ to the disturbances of the position vectors the relation $\hat{B} = \hat{R}^T \hat{G}$ is chosen as a starting

point. For ΔB this yields:

$$\begin{aligned}\Delta B &= (\hat{R} + \Delta R)^T (\hat{G} + \Delta G) - \hat{R}^T \hat{G} \\ &= \Delta R^T \hat{G} + \hat{R}^T \Delta G + \Delta R^T \Delta G.\end{aligned}\quad (6.6)$$

For small disturbances the last (quadratic) term is negligible. Besides, ΔB must be symmetrical. Requiring $\Delta B = \Delta B^T$ results in:

$$\hat{B}(\hat{R}^T \Delta R) - (\Delta R^T \hat{R})\hat{B} = \hat{R}^T \Delta G - \Delta G^T \hat{R} \quad (6.7)$$

where the right hand side is a skew-symmetrical matrix. Let Δx be the axial vector of this matrix, so

$$(\hat{R}^T \Delta G - \Delta G^T \hat{R})\mathbf{w} = \Delta x * \mathbf{w} \text{ for each } \mathbf{w}. \quad (6.8)$$

Using (6.1) for ΔG this axial vector can be written as a function of $\Delta \mathbf{p}_1, \Delta \mathbf{p}_2, \dots, \Delta \mathbf{p}_m$:

$$\Delta x = \frac{1}{m} \sum_{i=1}^m ((\mathbf{a}_i - \mathbf{a}) * (\hat{R}^T (\Delta \mathbf{p}_i - \Delta \mathbf{p}))). \quad (6.9)$$

Combining (6.5) and (6.8) with (6.7) it is easily seen that for each vector \mathbf{w} the following relation must hold:

$$\hat{B}(\Delta \mathbf{v} * \mathbf{w}) + \Delta \mathbf{v} * (\hat{B} \mathbf{w}) = \Delta x * \mathbf{w}. \quad (6.10)$$

From this equation $\Delta \mathbf{v}$ can be determined. The derivation is given in Appendix D and results in:

$$\Delta \mathbf{v} = \frac{1}{\hat{v}} \sum_{j=1}^3 (\hat{\gamma}_j \hat{\mathbf{n}}_j \hat{\mathbf{n}}_j^T) \Delta x = \frac{1}{\hat{v}} \hat{C} \Delta x \quad (6.11)$$

where $\hat{v}, \hat{\gamma}_1, \hat{\gamma}_2$ and $\hat{\gamma}_3$ were introduced before. Hence, component Δv_j of $\Delta \mathbf{v}$ in the direction of eigenvector $\hat{\mathbf{n}}_j$ ($j = 1, 2, 3$) is related to component Δx_j of Δx in that direction by:

$$\hat{v} \Delta v_j = \hat{\gamma}_j \Delta x_j \quad \text{for } j = 1, 2, 3 \quad (6.12)$$

where the components Δx_j ($j = 1, 2, 3$) of Δx are related to the disturbances $\Delta \mathbf{p}_1, \Delta \mathbf{p}_2, \dots, \Delta \mathbf{p}_m$ by (6.9). The factor $(\hat{v})^{-1} \hat{\gamma}_j$ in (6.12) can be considered as an amplification factor for Δx_j . The maximum amplification will occur in the direction of eigenvector $\hat{\mathbf{n}}_1$ with amplification factor $f_{\max} = (\hat{v})^{-1} \hat{\gamma}_1$. For an acceptable measurement this factor can be approximated by

$$f_{\max} \approx \frac{1}{\alpha_2 + \alpha_3} = \frac{1}{\text{tr}(A) - \alpha_1} \quad (6.13)$$

and it can be concluded that the sensitivity of the rotation matrix \hat{R} for disturbances in the measured position vectors of the markers is determined completely by the marker distribution.

The disturbance Δs of the factor \hat{s} follows from (3.15):

$$\Delta s \text{tr}(A) = \text{tr}(\Delta B) \quad (6.14)$$

where ΔB is given by (6.6). Again neglecting the quadratic term $\Delta R^T \Delta G$ it follows

$$\begin{aligned}\Delta s \text{tr}(A) &= \text{tr}(\hat{R}^T \Delta G) \\ &= \frac{1}{m} \sum_{i=1}^m [(\mathbf{a}_i - \mathbf{a})^T \hat{R}^T (\Delta \mathbf{p}_i - \Delta \mathbf{p})].\end{aligned}\quad (6.15)$$

SOME COMMENTS ON THE FINITE HELICAL AXIS

As mentioned before it is possible to write the components of the rotation matrix as a function of three independent variables, for instance Euler angles or Cardan angles. However, these angles are difficult to interpret and in biomechanical literature it is common practice to use so-called Euler parameters. Then the rotation of the body is considered as a rotation through an angle $\hat{\phi}$ about the so-called finite helical axis. Let $\hat{\mathbf{n}}$ be a unit vector along this axis, i.e. $\hat{\mathbf{n}}^T \hat{\mathbf{n}} = 1$. The sense of $\hat{\mathbf{n}}$ and of $\hat{\phi}$ correspond with the right-hand screw rule and ϕ will be non-negative and less than or equal to π rad, so $0 \leq \hat{\phi} \leq \pi$. The relation between the rotation matrix \hat{R} on the one hand and $\hat{\mathbf{n}}$ and $\hat{\phi}$ on the other hand is given by the requirement that

$$\hat{R}\mathbf{v} = (\hat{\mathbf{n}}^T \mathbf{v})\hat{\mathbf{n}} - \cos \hat{\phi} \hat{\mathbf{n}} * (\hat{\mathbf{n}} * \mathbf{v}) + \sin \hat{\phi} \mathbf{v} \quad (7.1)$$

holds for each vector \mathbf{v} [Chadwick (1976), Wittenburg (1977)].

A disadvantage of the description of the rotation in terms of $\hat{\mathbf{n}}$ and $\hat{\phi}$ is that $\hat{\mathbf{n}}$ is undefined if $\hat{R} = I$. If $\hat{R} \neq I$ both $\hat{\mathbf{n}}$ and $\hat{\phi}$ are unique and can be determined for given R [Spoor and Veldpaus (1980)]. Here only the sensitivity of $\hat{\mathbf{n}}$ and $\hat{\phi}$ for disturbances in the measured position vectors of the markers is considered. If $\hat{R} \neq I$ and $\Delta \mathbf{n}$ is small then $\hat{\mathbf{n}}$ and $\Delta \mathbf{n}$ are orthogonal. Starting from (7.1) a lengthy but straight forward derivation yields that $\Delta \mathbf{n}$ and $\Delta \phi$ are related to the axial vector $\Delta \mathbf{v}$ of $\hat{R}^T \Delta R$ by:

$$\hat{\mathbf{n}} \Delta \phi + \sin \phi \Delta \mathbf{n} - (1 - \cos \phi) \hat{\mathbf{n}} * \Delta \mathbf{n} = \Delta \mathbf{v}. \quad (7.2)$$

Multiplication by $\hat{\mathbf{n}}^T$ results in a relation for $\Delta \phi$,

$$\Delta \phi = \hat{\mathbf{n}}^T \Delta \mathbf{v} \quad (7.3)$$

while after some calculations it is found that:

$$\Delta \mathbf{n} = \frac{1}{2} \hat{\mathbf{n}} * \left[\Delta \mathbf{v} - \frac{1}{\tan \frac{\hat{\phi}}{2}} \hat{\mathbf{n}} * \Delta \mathbf{v} \right]. \quad (7.4)$$

This implies that $\hat{\mathbf{n}}$ is extremely sensitive to disturbances if $\hat{\phi}$ is small. Therefore the finite helical axis concept has doubtful utility for the description of small rotations, unless the noise level is sufficiently low (Woltring *et al.*, 1985).

SOME REMARKS ON THE PLANAR CASE

In general the motion of the considered body is three-dimensional and, as a consequence, the direction vector \mathbf{n} of the helical axis is unknown *a priori*. However, the experimental set-up for an acceptable measurement of the spatial co-ordinates of the markers is much more complex than the necessary set-up in the planar case. However, it is in many biomechanical situations quite acceptable to approximate the real motion of the body by a planar motion, consisting of an unknown rotation ϕ around an axis with known direction vector \mathbf{n} and a translation in the plane normal

to this axis. Then only the projections of the marker co-ordinates onto this plane have to be measured. In this section the planar case is considered in more detail. The essential differences with the preceding analysis are that now the direction vector \mathbf{n} of the helical axis is known *a priori* and that the position vectors \mathbf{a}_i and $\hat{\mathbf{p}}_i$ ($i = 1, 2, \dots, m$) have no component in the direction of \mathbf{n} , i.e.

$$\mathbf{a}_i^T \mathbf{n} = \hat{\mathbf{p}}_i^T \mathbf{n} = 0 \quad \text{for } i = 1, 2, \dots, m. \quad (8.1)$$

From the definition of the mean vectors \mathbf{a} and $\hat{\mathbf{p}}$ and of the matrices A , \hat{G} and \hat{P} it is seen that

$$\mathbf{a}^T \mathbf{n} = \hat{\mathbf{p}}^T \mathbf{n} = 0 \quad (8.2)$$

$$H \mathbf{n} = H^T \mathbf{n} = 0 \quad \text{for } H = A, \hat{G} \text{ or } \hat{P}. \quad (8.3)$$

Due to the fact that \mathbf{n} is known the rotation matrix \hat{R} , as specified by (7.1), only depends on the unknown rotation $\hat{\phi}$ and it is easily seen that $\hat{R}^T \hat{R} = I$ and $\det(\hat{R}) = 1$ for all values of $\hat{\phi}$. Using these results in (3.12) the least squares function f is seen to depend on \hat{s} , $\hat{\mathbf{r}}$ and $\hat{\phi}$ only and is given by:

$$f(\hat{s}, \hat{\mathbf{r}}, \hat{\phi}) = (\hat{\mathbf{p}} - \mathbf{a} - \hat{\mathbf{r}})^T (\hat{\mathbf{p}} - \mathbf{a} - \hat{\mathbf{r}}) + \text{tr}(\hat{P} - 2\hat{s}\hat{G}\hat{R}^T(\hat{\phi}) + \hat{s}^2 A). \quad (8.4)$$

This function must be minimized under the remaining constraint condition

$$\hat{s} > 0. \quad (8.5)$$

An elaboration of this requirement results in the relations

$$\hat{\mathbf{r}} = \hat{\mathbf{p}} - \mathbf{a} \quad (8.6)$$

$$\hat{s} \text{tr}(A) = \text{tr}(\hat{G}\hat{R}^T) = \text{tr}(\hat{G}^T \hat{R}) \quad (8.7)$$

$$\text{tr}\left(\hat{G} \frac{d\hat{R}}{d\phi}\right) = 0, \quad (8.8)$$

and, because \hat{s} must be positive while $\text{tr}(A)$ is positive, it follows that

$$\text{tr}(\hat{G}^T \hat{R}) > 0, \quad (8.9)$$

must hold. With the definition of \hat{G} and the specification (7.1) of \hat{R} the last two equations can be rewritten, yielding:

$$\cos \hat{\phi} \mathbf{n}^T \hat{\mathbf{x}} = \sin \hat{\phi} \text{tr}(\hat{G}) \quad (8.10)$$

$$\cos \hat{\phi} \text{tr}(\hat{G}) + \sin \hat{\phi} \mathbf{n}^T \hat{\mathbf{x}} > 0 \quad (8.11)$$

where the vector $\hat{\mathbf{x}}$ is given by

$$\hat{\mathbf{x}} = \frac{1}{m} \sum_{i=1}^m [(\mathbf{a}_i - \mathbf{a}) * (\hat{\mathbf{p}}_i - \hat{\mathbf{p}})]. \quad (8.12)$$

By these equations the angle $\hat{\phi}$ is determined uniquely. After calculation of $\hat{\phi}$ the quantities \hat{s} and $\hat{\mathbf{r}}$ can be found from (8.7) and (8.6). In general the calculated value of \hat{s} will differ from the exact value 1. Neglecting numerical errors the difference is caused partly by measurement errors but also—and in most cases this is the main reason—by the fact that the real motion is not planar. As a consequence, the difference $\hat{s} - 1$ will give

some indication about the validity of the assumption that this motion is planar. Therefore it is advisable to determine \hat{s} whenever this assumption is used, especially because the extra amount of calculation time is very small.

DISCUSSION

The derivations in the preceding sections are rather lengthy but the final algorithms for the calculation of the translation vector $\hat{\mathbf{r}}$, the rotation matrix \hat{R} and the scaling factor \hat{s} are quite simple. No initial estimates for these quantities are needed and no numerical problems will arise if the marker distribution is spatial or at least planar. Moreover, the algorithms are optimal in the least-squares sense, as opposed to other algorithms as described by Schut (1963) and Conati (1977).

In this paper the factor \hat{s} is unknown *a priori*. The results may be easily adapted to the case of an *a priori* known factor \hat{s} , especially to the isometric case where $\hat{s} = 1$. Then relation (3.15) becomes obsolete but the formulae (3.14) and (3.16) for $\hat{\mathbf{r}}$ and \hat{R} remain the same and subroutine POLDEC (see Appendix E) can be applied without any modification. In practical applications it is suggested to choose \hat{s} *a priori* unknown because the calculated value of \hat{s} can give some information about the quality of the measurement.

For the calculation of $\hat{\mathbf{r}}$, \hat{R} and \hat{s} a least-squares criterion was adopted, since this results in mathematically tractable formulae. It depends on the measurement situation at hand whether the unweighted criterion, used here, is statistically optimal. For example this may be the case when performing stereotactic measurements on an *in vitro* preparation but not necessarily in a stereophotogrammetric context where depth errors on individual markers may be considerably larger than errors in the plane normal to the depth direction. In the latter case it may be useful to revert to iterative approaches (Miller *et al.*, 1981; Woltring, 1982), which do not require explicit reconstruction of the spatial marker co-ordinates. Instead, these approaches rely directly on the image co-ordinates (of at least three non-collinear markers) which are not necessarily available from more than one camera per marker. Such generalized, iterative approaches require suitable initialization procedures and do not always yield unique estimates. The present algorithm may serve the initialization purpose, in combination with an explicit marker reconstruction procedure such as the ODLE-algorithm (Woltring, 1980).

It has been shown that the sensitivity of the calculated quantities $\hat{\mathbf{r}}$, \hat{R} and \hat{s} for disturbances in the measured position vectors of the markers is determined largely by the marker distribution. The results of the analysis can serve as a means for assessing the quality of a given marker distribution. These results are formulated in terms of the eigenvalues of the so-called distribution matrix A and it turns out that

at least two of these eigenvalues must differ significantly from zero.

The finite helical axis is shown to be unsuitable for the description of small rotations from noisy marker coordinate measurements (cf. Woltring *et al.*, 1985). If the motion of the body has to be described by means of measurements of the marker co-ordinates at a number of points of time $t_1, t_2, t_3 \dots$ it is preferable to smooth and fit the raw measurement data to a continuous model, yielding the translation vector $\hat{\mathbf{r}}(t_i)$, the rotation matrix $\hat{\mathbf{R}}(t_i)$ and the factor $\hat{s}(t_i)$ of the body at time t_i with respect to the body at time t_1 . A similar approach was outlined earlier by Woltring *et al.* (1986).

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APPENDIX A: STATIONARY VALUES OF THE MODIFIED LEAST SQUARES FUNCTION

The modified least squares function $F = F(\hat{s}, \hat{\mathbf{r}}, \hat{\mathbf{R}}, L)$, defined by (3.11) and (3.13), is stationary if the first variation δF of F is zero for each infinitesimally small variation δs , $\delta \mathbf{r}$, $\delta \mathbf{R}$ and δL of the variables \hat{s} , $\hat{\mathbf{r}}$, $\hat{\mathbf{R}}$ and L , where δF is defined by

$$\delta F = F(\hat{s} + \delta s, \hat{\mathbf{r}} + \delta \mathbf{r}, \hat{\mathbf{R}} + \delta \mathbf{R}, L + \delta L) - F(\hat{s}, \hat{\mathbf{r}}, \hat{\mathbf{R}}, L). \quad (\text{A.1})$$

First, variations of L are considered. Then δF is given by

$$\delta F = -\text{tr}((\hat{\mathbf{R}}^T \hat{\mathbf{R}} - \mathbf{I}) \delta L). \quad (\text{A.2})$$

Requiring $\delta F = 0$ for each δL results in the constraint condition

$$\hat{\mathbf{R}}^T \hat{\mathbf{R}} = \mathbf{I}. \quad (\text{A.3})$$

Next, variations of $\hat{\mathbf{r}}$ are considered. From

$$\delta F = -2(\hat{\mathbf{p}} - \hat{\mathbf{r}} - \mathbf{a})^T \delta \mathbf{r} \quad (\text{A.4})$$

it is easily seen that $\delta F = 0$ for each $\delta \mathbf{r}$ if

$$\hat{\mathbf{r}} = \hat{\mathbf{p}} - \mathbf{a}. \quad (\text{A.5})$$

Furthermore, variation of \hat{s} results in

$$\delta F = -2\text{tr}(\hat{\mathbf{G}} \hat{\mathbf{R}}^T - \hat{s} \hat{\mathbf{R}} \hat{\mathbf{A}} \hat{\mathbf{R}}^T) \delta s. \quad (\text{A.6})$$

Using (A.6) and requiring $\delta F = 0$ for each δs yields:

$$\hat{s} \text{tr}(\hat{\mathbf{R}} \hat{\mathbf{A}} \hat{\mathbf{R}}^T) = \text{tr}(\hat{\mathbf{G}} \hat{\mathbf{R}}^T). \quad (\text{A.7})$$

Finally, variations of $\delta \mathbf{R}$ are considered. Using (A.1) it is seen that

$$\delta F = \text{tr}(-2\hat{s}\hat{\mathbf{G}}\delta\mathbf{R}^T + \hat{s}^2\delta\mathbf{R}\hat{\mathbf{A}}\hat{\mathbf{R}}^T + \hat{s}^2\hat{\mathbf{R}}\hat{\mathbf{A}}\delta\mathbf{R}^T - \delta\mathbf{R}^T\hat{\mathbf{R}}L - \hat{\mathbf{R}}^T\delta\mathbf{R}L). \quad (\text{A.8})$$

This relation can be simplified by employing the identities

$$\begin{aligned} \text{tr}(\delta\mathbf{R}\hat{\mathbf{A}}\hat{\mathbf{R}}^T) &= \text{tr}(\hat{\mathbf{R}}\hat{\mathbf{A}}^T\delta\mathbf{R}^T) \\ \text{tr}(\delta\mathbf{R}^T\hat{\mathbf{R}}L + \hat{\mathbf{R}}^T\delta\mathbf{R}L) &= \text{tr}(\hat{\mathbf{R}}(L + L^T)\delta\mathbf{R}^T). \end{aligned} \quad (\text{A.9})$$

Substitution in (A.8) and requiring $\delta F = 0$ for each $\delta \mathbf{R}$ results in

$$\hat{\mathbf{G}} = \hat{\mathbf{R}}\hat{\mathbf{B}}; \quad \hat{\mathbf{B}} = \hat{s}\mathbf{A} - \frac{1}{2\hat{s}}(L + L^T). \quad (\text{A.10})$$

Hence, (A.7) can be written as

$$\hat{s} \text{tr}(\hat{\mathbf{R}}\hat{\mathbf{A}}\hat{\mathbf{R}}^T) = \text{tr}(\hat{\mathbf{R}}\hat{\mathbf{B}}\hat{\mathbf{R}}^T)$$

and from $\hat{\mathbf{R}}^T \hat{\mathbf{R}} = \mathbf{I}$ and the identity $\text{tr}(\hat{\mathbf{R}}\hat{\mathbf{D}}\hat{\mathbf{R}}^T) = \text{tr}(\hat{\mathbf{D}}\hat{\mathbf{R}}^T\hat{\mathbf{R}}) = \text{tr}(\hat{\mathbf{D}})$, holding for every matrix $\hat{\mathbf{D}}$, it is readily seen that

$$\hat{s} \text{tr}(\mathbf{A}) = \text{tr}(\hat{\mathbf{B}}). \quad (\text{A.11})$$

The equations (A.5), (A.10) and (A.11) correspond with the equations (3.9), (3.14), (3.17) and (3.15) respectively.

APPENDIX B: THE ADJOINT OF A 3*3 MATRIX

The adjoint D^a of a 3*3 matrix D is uniquely determined by the requirement that for each vector \mathbf{v} and \mathbf{w} must hold (Chadwick, 1976):

$$(D\mathbf{v}) * (D\mathbf{w}) = D^a(\mathbf{v} * \mathbf{w}), \quad (\text{B.1})$$

where $*$ is the vector product operator. From this definition it is seen that

$$(DH\mathbf{v}) * (DH\mathbf{w}) = D^a((H\mathbf{v}) * (H\mathbf{w})) = D^a H^a(\mathbf{v} * \mathbf{w}). \quad (\text{B.2})$$

Hence, the adjoint of the matrix product DH is equal to the product of the adjoint matrices D^a and H^a :

$$(DH)^a = D^a H^a. \quad (\text{B.3})$$

According to Chadwick (1976) the determinant of any matrix D , $\det(D)$, can be determined from the requirement

$$\det(D)\mathbf{v} * \mathbf{w} = D^T(D\mathbf{v}) * (D\mathbf{w}) = D^T D^a(\mathbf{v} * \mathbf{w}) \quad (\text{B.4})$$

which holds for all vectors \mathbf{v} and \mathbf{w} . This results in the conclusion that

$$D^T D^a = \det(D)I. \quad (\text{B.5})$$

Therefore, the adjoint R^a of a rotation matrix R is equal to R itself.

For a given matrix D the adjoint D^a can be calculated very quickly. Let \mathbf{d}_1 , \mathbf{d}_2 and \mathbf{d}_3 be the columns of D . Then one may verify by inspection that the columns of D^a are equal to $\mathbf{d}_2 * \mathbf{d}_3$, $\mathbf{d}_3 * \mathbf{d}_1$ and $\mathbf{d}_1 * \mathbf{d}_2$. In other words, if D is written as

$$D = [\mathbf{d}_1 \ \mathbf{d}_2 \ \mathbf{d}_3] \quad (\text{B.6})$$

then D^a can be determined from

$$D^a = [\mathbf{d}_2 * \mathbf{d}_3 \ \mathbf{d}_3 * \mathbf{d}_1 \ \mathbf{d}_1 * \mathbf{d}_2]. \quad (\text{B.7})$$

APPENDIX C. AN ITERATIVE METHOD TO DETERMINE β_1 AND β_2

The non-linear equations (4.12) can be written as:

$$x^2 - 2h_1 y - 1 = 0; \quad y^2 - 2h_2 x - 1 = 0 \quad (\text{C.1})$$

where the known quantities h_1 and h_2 and the unknown quantities x and y are given by:

$$h_1 = \frac{\hat{g}_2}{\hat{g}_1^2}, \quad h_2 = \frac{\hat{g}_1 \hat{g}_3}{\hat{g}_2^2}; \quad x = \frac{\hat{\beta}_1}{\hat{g}_1}, \quad y = \frac{\hat{\beta}_2}{\hat{g}_2}. \quad (\text{C.2})$$

The equations (C.1) can be solved iteratively, using the Newton-Raphson method. Let x_n and y_n be the approximations for the solution of (C.1), obtained in iteration step n . Then new approximations x_{n+1} and y_{n+1} follow from

$$x_{n+1} = x_n + \Delta x_n; \quad y_{n+1} = y_n + \Delta y_n \quad (\text{C.3})$$

where the corrections Δx_n and Δy_n are given by:

$$\begin{bmatrix} \Delta x_n \\ \Delta y_n \end{bmatrix} = \frac{1}{2d_n} \begin{bmatrix} y_n h_1 \\ h_2 x_n \end{bmatrix} \begin{bmatrix} 1 - x_n^2 + 2h_1 y_n \\ 1 - y_n^2 + 2h_2 x_n \end{bmatrix}; \quad d_n = x_n y_n - h_1 h_2. \quad (\text{C.4})$$

With the initial guess $x_0 = y_0 = 1$ it can be shown that, for an acceptable set of measurements, in each iteration step n will hold $x_n > 0$, $y_n > 0$ and $d_n > 0$. The convergence of this iteration process is locally quadratic and the initial guess $x_0 = y_0 = 1$ is fairly accurate for any acceptable set of measurements. Hence, only a few iteration steps are necessary.

APPENDIX D: DETERMINATION OF $\Delta \mathbf{v}$ AS A FUNCTION OF $\Delta \mathbf{x}$

The vector $\Delta \mathbf{v}$ has to be solved from (6.10), i.e. from

$$\hat{B}(\Delta \mathbf{v} * \mathbf{v}) + \Delta \mathbf{v} * (\hat{B} \mathbf{v}) = \Delta \mathbf{x} * \mathbf{v} \quad \text{for each } \mathbf{v}. \quad (\text{D.1})$$

The left hand side of this equation can be rewritten, using the definition of the trace of a matrix. It can be shown (Chadwick, 1976) that

$$\text{tr}(D) \mathbf{w} * \mathbf{v} = D^T(\mathbf{w} * \mathbf{v}) + (D \mathbf{w}) * \mathbf{v} + \mathbf{w} * (D \mathbf{v}) \quad (\text{D.2})$$

holds for every D , \mathbf{v} and \mathbf{w} . Replacing D by $\hat{B} = \hat{B}^T$ and \mathbf{w} by $\Delta \mathbf{v}$ yields:

$$\hat{B}(\Delta \mathbf{v} * \mathbf{v}) + \Delta \mathbf{v} * (\hat{B} \mathbf{v}) = [(\text{tr}(\hat{B})I - \hat{B})\Delta \mathbf{v}] * \mathbf{v}. \quad (\text{D.3})$$

Combining this result with (D.1) gives

$$[\text{tr}(\hat{B})I - \hat{B}]\Delta \mathbf{v} = \Delta \mathbf{x} \quad (\text{D.4})$$

and using (4.3), (4.5) and (5.2) it is seen that

$$\sum_{j=1}^3 [\hat{v}(\hat{g}_j)^{-1} \hat{\mathbf{n}}_j \hat{\mathbf{n}}_j^T] \Delta \mathbf{v} = \Delta \mathbf{x}. \quad (\text{D.5})$$

This immediately results in equation (6.11).

APPENDIX E: THE FORTRAN SUBROUTINE POLDEC

In the following subroutine some lines contain braced statements. These statements represent standard processes and are not given in more detail.

Furthermore a subroutine ADJOIN is included in which the adjoint of a 3×3 matrix is calculated as depicted in Appendix B.

```

SUBROUTINE POLDEC(G,R,B,IRANK)
  DIMENSION G(3,3), R(3,3), B(3,3), AD(3,3),
  P(3,3), PAD(3,3)
  DOUBLE PRECISION G,R,B,BETA1,BETA2,
  BETA3,AD,P,J1,J2,J3,X,Y,
  * DET,DX,DY,DETG,HELP1,HELP2,
  * EPS,PAD,H1,H2
  INTEGER*2 IRANK
  C global parameters: G = RB and rank IRANK of G
  C calculation of the adjoint of G
  CALL ADJOIN(G,AD)
  C calculation of det(G)
  DETG = G(1,1)*AD(1,1)+G(2,1)*AD(2,1)
  +G(3,1)*AD(3,1)
  {calculation of the matrix P = GTG}
  C calculation of the invariants J1, J2 and J3 of
  C P = GTG
  J1 = P(1,1)+P(2,2)+P(3,3)
  CALL ADJOIN(P,PAD)
  J2 = PAD(1,1)+PAD(2,2)+PAD(3,3)
  J3 = DETG*DETG
  C test for the rank of the matrix G through param-
  C eter EPS
  EPS = 1.D-12
  IRANK = 0
  IF (J3.GT.EPS) IRANK = 3
  IF ((IRANK.NE.3).AND.(J2.GT.EPS))
  IRANK = 2
  IF ((IRANK.EQ.0).AND.(J1.GT.EPS))
  IRANK = 1
  C if IRANK less than 2: no decomposition possible
  IF (IRANK.LT.2) GOTO 1000
  C calculation of the invariants BETA1, BETA2 and
  C BETA3 of B by
  C means of the NEWTON-RAPHSON method
  C the tolerance for convergence is given in het
  C parameter EPS
  EPS = 1.D-10
  X = 1.D0
  Y = 1.D0
  H1 = DSQRT(J2)/J1
  H2 = DETG*DSQRT(J1)/J2
  C start of the iteration loop
  100 DET = X*Y-H1*H2
  HELP1 = 0.5D0*(1.D0-X*X+2.D0*H1*Y)
  HELP2 = 0.5D0*(1.D0-Y*Y+2.D0*H2*X)
  DX = (Y*HELP1+H1*HELP2)/DET
  DY = (H2*HELP1+X*HELP2)/DET
  IF ((DX*DX/(X*X)+DY*DY/(Y*Y)).LT.EPS)
  GOTO 200
  X = X+DX
  Y = Y+DY
  GOTO 100
  200 X = X+DX
  Y = Y+DY
  C end of the iteration loop
  BETA1 = X*DSQRT(J1)
  BETA2 = Y*DSQRT(J2)
  BETA3 = DETG
  C calculation of R and B
  {calculation of (BETA1*G+AD) and
  {P+BETA2*I}}
  {inversion of (P+BETA2*I)}
  {calculation of R from R = (BETA1*G+AD)
  (P+BETA2*I)-1}

```

```

1000 {calculation of B from  $B = R^T G$ }
      RETURN
      END

      SUBROUTINE ADJOIN (G,GAD)
      DIMENSION G(3,3), GAD (3,3)
      DOUBLE PRECISION G, GAD
      in this routine the adjoint  $GAD$  of  $G$  is calculated
      GAD(1,1) = G(2,2)*G(3,3) - G(3,2)*G(2,3)
      GAD(2,1) = G(3,2)*G(1,3) - G(1,2)*G(3,3)
      GAD(3,1) = G(1,2)*G(2,3) - G(2,2)*G(1,3)
      GAD(1,2) = G(2,3)*G(3,1) - G(3,3)*G(2,1)
      GAD(2,2) = G(3,3)*G(1,1) - G(1,3)*G(3,1)
      GAD(3,2) = G(1,3)*G(2,1) - G(2,3)*G(1,1)
      GAD(1,3) = G(2,1)*G(3,2) - G(3,1)*G(2,2)
      GAD(2,3) = G(3,1)*G(1,2) - G(1,1)*G(3,2)
      GAD(3,3) = G(1,1)*G(2,2) - G(2,1)*G(1,2)
      RETURN
      END.
C

```