

Unphysical properties of the rotation tensor estimated by least squares optimization with specific application to biomechanics

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Abstract

Analysis of the transformation of one data set into another is a ubiquitous problem in many fields of science. Many works approximate the transformation of a reference cluster of n vectors \mathbf{X}_i ($i=1,2,\dots,n$) into another cluster of n vectors \mathbf{x}_i by a translation and a rotation using a least squares optimization to obtain the rotation tensor \mathbf{Q} . The objective of this work is to prove that this rotation tensor \mathbf{Q} exhibits unphysical dependence on the shape and orientation of the reference cluster. In contrast, when the transformation is approximated by a translation and a general non-singular tensor \mathbf{F} , which includes deformations, then the associated rotation tensor \mathbf{R} does not exhibit these unphysical properties. An example in biomechanics quantifies the errors of these unphysical properties.

Keywords: anthropometric scaling; biomechanical motion analysis; factor structure; least squares; polar decomposition; registration of shapes; satellite attitude; soft tissue artifact

1. Introduction

Analysis of the transformation of one data set into another is a ubiquitous problem in many fields of science. For examples: behavioral science analysis (Hurley and Catell, 1962; Schonemann, 1966); satellite attitude estimation (Wahba, 1966); registration and motion of 3-D shapes (Laub and Shiflett, 1982; Arun et al., 1987; Besl and McKay, 1992); anthropometric scaling (Lew and Lewis, 1977; Sommer et al., 1982); and biomechanical motion analysis (Spoor and Veldpaus, 1980; Veldpaus et al., 1988; Soderkvist and Wedin, 1993; Challis, 1995; Cappozzo et al., 1996; Ball and Pierrynowski, 1998; Cappozzo et al. 2005; Dumas and Cheze, 2009), with specific treatment of the Soft Tissue Artifact (STA) limiting the determination of the underlying bone position and orientation (pose) from markers placed on the surface of soft tissues (Leardini et al., 2005; Dumas and Cheze, 2009; Peters et al., 2010).

For biomechanical motion analysis it is common to place a cluster of n markers on the skin at various points of the body. Measurements are made of the positions \mathbf{X}_i ($i=1,2,\dots,n$) of these markers in a specified reference configuration and their positions \mathbf{x}_i as a function of time (Cappozzo et al., 2005). This cluster of markers is analyzed to estimate the pose of the underlying bone segment. Muscle activation, inertial effects and deformations of the soft tissues associated with the STA cause uncertainty in the bone pose that limits accurate estimation of forces and moments applied to various joints (Cappozzo et al., 1996; Leardini et al., 2005; Peters et al., 2010).

In the applications discussed above the vectors \mathbf{x}_i include inhomogeneous deformations relative to \mathbf{X}_i due to a number of sources associated with measurement error and actual inhomogeneous deformations. Specifically, in biomechanical motion analysis the forces and moments on body joints can be estimated by knowing the rigid motion of bones in the body. However, piercing the skin by placing pins in the bone to determine actual bone position cannot be done for general patient diagnosis. Therefore, estimates of the bone pose using markers on the deformable skin are essential.

From a continuum mechanics point of view, it is obvious that the rotation of a material line element in a deformable body depends on the deformation field and on the specific orientation of the line element in the reference configuration. If the deformations are not

too large then it is reasonable to use a rigid body approximation. Often (e.g., Schonemann, 1966; Wahba, 1966; Spoor and Veldpaus, 1980; Arun et al., 1987; Veldpaus et al., 1988; Besl and McKay, 1992; Soderkvist and Wedin, 1993; Challis, 1995) the transformation of \mathbf{X}_i into \mathbf{x}_i is approximated as a translation and rotation using least squares optimization to determine the rotation tensor \mathbf{Q} . The main objective of this work is to prove that this rotation tensor \mathbf{Q} exhibits an unphysical dependence on the orientation and shape of the reference cluster \mathbf{X}_i . In contrast, when the transformation between these data sets is approximated by a translation and a general non-singular tensor \mathbf{F} , which includes deformations, then the associated rotation tensor \mathbf{R} is uninfluenced by shape and orientation changes of the reference cluster. For biomechanical motion analysis this means that the estimates of the underlying bone pose using \mathbf{Q} will include errors due the STA as well as additional unphysical errors which depend on the placement of the markers. These additional unphysical errors can be removed using the analysis based on \mathbf{F} .

2. The affine approximation

Within a general context, the objective is to determine a simple approximate relationship between the reference cluster of vectors \mathbf{X}_i and another cluster of vectors \mathbf{x}_i . To this end, it is convenient to define the centroids $\{\mathbf{X}, \mathbf{x}\}$ of $\{\mathbf{X}_i, \mathbf{x}_i\}$ by the expressions

$$\mathbf{X} = \frac{1}{n} \sum_{i=1}^n \mathbf{X}_i, \quad \mathbf{x} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i, \quad (2.1)$$

and define the difference vectors, $\Delta\mathbf{X}_i$ and $\Delta\mathbf{x}_i$, such that

$$\mathbf{X}_i = \mathbf{X} + \Delta\mathbf{X}_i, \quad \mathbf{x}_i = \mathbf{x} + \Delta\mathbf{x}_i. \quad (2.2)$$

Then, the estimates \mathbf{x}_i^* of \mathbf{x}_i based on an affine transformation of \mathbf{X}_i are defined by

$$\mathbf{x}_i^* = \mathbf{X} + \mathbf{t} + \mathbf{F}\Delta\mathbf{X}_i, \quad (2.3)$$

where \mathbf{t} is the approximate translation vector of \mathbf{X} and \mathbf{F} is a second order non-singular transformation tensor.

Using a least squares procedure with an affine approximation (2.3), define the function of the sum of squared errors (e.g. Plackett, 1960)

$$f(\mathbf{t}, \mathbf{F}) = \sum_{i=1}^n (\mathbf{x}_i - \mathbf{x}_i^*) \cdot (\mathbf{x}_i - \mathbf{x}_i^*) = \sum_{i=1}^n [(\mathbf{x}_i - \mathbf{X}) - (\mathbf{t} + \mathbf{F}\Delta\mathbf{X}_i)] \cdot [(\mathbf{x}_i - \mathbf{X}) - (\mathbf{t} + \mathbf{F}\Delta\mathbf{X}_i)] , \quad (2.4)$$

where (\bullet) denotes the inner product between the vectors. If $\{\mathbf{X}_i, \mathbf{x}_i\}$ are vectors of dimension m , then \mathbf{t} has dimension m and \mathbf{F} has dimension $m \times m$. In continuum mechanics the vectors are in 3-space with $m=3$, $\Delta\mathbf{X}_i$ represent material line elements in the reference configuration, $\Delta\mathbf{x}_i$ represent material line elements in the present configuration and \mathbf{F} is called the deformation gradient. In the following discussion use will be made of the terms translation, deformation, rotation and stretch from continuum mechanics even though other names for the same mathematical quantities are used in other fields.

Substituting (2.2) into (2.4) yields

$$f(\mathbf{t}, \mathbf{F}) = n [(\mathbf{x} - \mathbf{X}) - \mathbf{t}] \cdot [(\mathbf{x} - \mathbf{X}) - \mathbf{t}] + \sum_{i=1}^n (\Delta\mathbf{x}_i - \mathbf{F}\Delta\mathbf{X}_i) \cdot (\Delta\mathbf{x}_i - \mathbf{F}\Delta\mathbf{X}_i) . \quad (2.5)$$

Next, taking the variation δf of $f(\mathbf{t}, \mathbf{F})$ with respect to the variations $\{\delta\mathbf{t}, \delta\mathbf{F}\}$ of $\{\mathbf{t}, \mathbf{F}\}$ yields

$$\delta f = -2n [(\mathbf{x} - \mathbf{X}) - \mathbf{t}] \cdot \delta\mathbf{t} - 2 \sum_{i=1}^n (\Delta\mathbf{x}_i \otimes \Delta\mathbf{X}_i - \mathbf{F}\Delta\mathbf{X}_i \otimes \Delta\mathbf{X}_i) \cdot \delta\mathbf{F} , \quad (2.6)$$

where $\mathbf{a} \otimes \mathbf{b}$ denotes the tensor (outer) product of the vectors $\{\mathbf{a}, \mathbf{b}\}$. Since $\delta\mathbf{t}$ and $\delta\mathbf{F}$ are independent, critical values of f are determined by the condition that the coefficients of $\{\delta\mathbf{t}, \delta\mathbf{F}\}$ vanish, which yields

$$\begin{aligned} \mathbf{t} &= \mathbf{x} - \mathbf{X} , \quad \Delta\mathbf{x}_i = \mathbf{F}\Delta\mathbf{X}_i , \\ \mathbf{F} &= \bar{\mathbf{F}}\mathbf{H}^{-1} , \quad \bar{\mathbf{F}} = \sum_{i=1}^n \Delta\mathbf{x}_i \otimes \Delta\mathbf{X}_i , \quad \mathbf{H} = \sum_{i=1}^n \Delta\mathbf{X}_i \otimes \Delta\mathbf{X}_i = \mathbf{H}^T , \end{aligned} \quad (2.7)$$

where $(^T)$ denotes the transpose operator and it has been assumed that the tensor \mathbf{H} is non-singular. It follows that \mathbf{t} is the translation of the centroids and it is noted that \mathbf{F} includes both rotation and stretching of $\Delta\mathbf{X}_i$ since the orientation and length of $\Delta\mathbf{x}_i$ can be different from those of $\Delta\mathbf{X}_i$.

Using a generalization of the polar decomposition theorem (Malvern, 1969) and assuming that \mathbf{F} has a positive determinant, \mathbf{F} can be represented in the form

$$\mathbf{F} = \mathbf{R}\mathbf{M} , \quad \mathbf{R}^T\mathbf{R} = \mathbf{I} , \quad \mathbf{M}^T = \mathbf{M} , \quad (2.8)$$

where \mathbf{R} is a unique proper orthogonal rotation tensor, \mathbf{M} is a unique positive definite, symmetric stretch tensor and \mathbf{I} is the identity tensor.

3. The rotation tensor based on the rigid body approximation

For the rotation tensor based on the rigid body approximation, \mathbf{F} in (2.3) is restricted to be a proper orthogonal rotation tensor \mathbf{Q} , which satisfies the conditions

$$\mathbf{Q}^T \mathbf{Q} = \mathbf{I}, \quad \delta \mathbf{Q} = \delta \boldsymbol{\Omega} \mathbf{Q}, \quad \delta \boldsymbol{\Omega}^T = -\delta \boldsymbol{\Omega}, \quad (3.1)$$

where $\delta \boldsymbol{\Omega}$ is a skew-symmetric tensor. In the general case, $\{\mathbf{Q}, \delta \boldsymbol{\Omega}\}$ both have dimensions $m \times m$.

The expressions (2.1)-(2.6) are valid for this case with $\{\mathbf{F}, \delta \mathbf{F}\}$ replaced by $\{\mathbf{Q}, \delta \mathbf{Q}\}$ so that with the help of (3.1) and (2.7), the expression (2.6) is written in the form

$$\delta f = -2n [(\mathbf{x} - \mathbf{X}) - \mathbf{t}] \cdot \delta \mathbf{t} - 2 (\bar{\mathbf{F}} \mathbf{Q}^T - \mathbf{Q} \mathbf{H} \mathbf{Q}^T) \cdot \delta \boldsymbol{\Omega}. \quad (3.2)$$

Since $\delta \boldsymbol{\Omega}$ is skew-symmetric and \mathbf{H} is symmetric, critical values of f require

$$\mathbf{t} = \mathbf{x} - \mathbf{X}, \quad \Delta \mathbf{x}_i = \mathbf{Q} \Delta \mathbf{X}_i, \quad \bar{\mathbf{F}} \mathbf{Q}^T = \mathbf{Q} \bar{\mathbf{F}}^T. \quad (3.3a,b)$$

Now, assuming that $\bar{\mathbf{F}}$ has a positive determinant, use can be made of the polar decomposition theorem to express $\bar{\mathbf{F}}$ in the form

$$\bar{\mathbf{F}} = \bar{\mathbf{R}} \bar{\mathbf{M}}, \quad \bar{\mathbf{R}}^T \bar{\mathbf{R}} = \mathbf{I}, \quad \bar{\mathbf{M}}^T = \bar{\mathbf{M}}, \quad (3.4)$$

where $\bar{\mathbf{R}}$ is a unique proper orthogonal rotation tensor and $\bar{\mathbf{M}}$ is a unique positive definite stretch tensor. It then follows that the unique solution of (3.3b) requires

$$\mathbf{Q} = \bar{\mathbf{R}}. \quad (3.5)$$

4. The rotation tensor based on the affine approximation

In Section 3 it was shown that when the least squares approximation is used together with the constraint that \mathbf{F} be a rotation tensor \mathbf{Q} , the optimal value of \mathbf{Q} is given by the rotation tensor $\bar{\mathbf{R}}$ associated with the polar decomposition of the auxiliary tensor $\bar{\mathbf{F}}$ defined in (2.7). An alternative specification of \mathbf{Q} can be obtained using the least squares optimization based on the affine approximation to obtain the tensor \mathbf{F} defined in (2.7).

Then, the value of \mathbf{Q} can be specified by the rotation tensor \mathbf{R} in the polar decomposition of \mathbf{F}

$$\mathbf{Q} = \mathbf{R} . \quad (4.1)$$

Next, using (2.7), (2.8) and (3.4) it follows that

$$\mathbf{RM} = \bar{\mathbf{R}}\bar{\mathbf{M}}\mathbf{H}^{-1} , \quad (4.2)$$

which proves that the rotation tensor \mathbf{R} is different from $\bar{\mathbf{R}}$ whenever $\bar{\mathbf{M}}\mathbf{H}^{-1}$ is not symmetric. This means that the solutions (3.5) and (4.1) are different, with the estimated rotation being influenced by deformations due to \mathbf{F} .

In order to quantify the influence of deformations on the estimate of the rotation tensor, it is noted that a general line element (i.e. vector) in the reference configuration with unit direction \mathbf{S} has stretch λ and is rotated to the unit direction \mathbf{s} in the present configuration, with

$$\begin{aligned} \lambda \mathbf{s} &= \mathbf{FS} = \mathbf{RMS} , \quad \mathbf{S} \cdot \mathbf{S} = 1 , \quad \mathbf{s} \cdot \mathbf{s} = 1 , \\ \lambda^2 &= \mathbf{FS} \cdot \mathbf{FS} = \mathbf{C} \cdot \mathbf{S} \otimes \mathbf{S} , \quad \mathbf{C} = \mathbf{F}^T \mathbf{F} = \mathbf{M}^2 , \end{aligned} \quad (4.3)$$

where $\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{AB}^T)$ is the inner product of two second order tensors $\{\mathbf{A}, \mathbf{B}\}$. It then follows that the angle γ between \mathbf{MS} and \mathbf{S} is given by

$$\cos \gamma = \frac{1}{\lambda} \mathbf{MS} \cdot \mathbf{S} . \quad (4.4)$$

Since \mathbf{S} is a unit vector its variation $\delta \mathbf{S}$ can be expressed in the form

$$\delta \mathbf{S} = \delta \mathbf{\Omega} \mathbf{S} , \quad \delta \mathbf{\Omega}^T = -\delta \mathbf{\Omega} , \quad (4.5)$$

where $\delta \mathbf{\Omega}$ is an arbitrary skew-symmetric tensor. Now, for fixed \mathbf{M} the variation of (4.4) yields

$$-\sin \phi \delta \gamma = \frac{1}{\lambda} \mathbf{A} \cdot \delta \mathbf{\Omega} , \quad (4.6)$$

which vanishes for all $\delta \mathbf{\Omega}$ provided that the skew-symmetric tensor \mathbf{A} vanishes

$$\mathbf{A} = \mathbf{M}(\mathbf{S} \otimes \mathbf{S}) - (\mathbf{S} \otimes \mathbf{S})\mathbf{M} - \frac{1}{2\lambda^2} (\mathbf{M} \cdot \mathbf{S} \otimes \mathbf{S}) [\mathbf{C}(\mathbf{S} \otimes \mathbf{S}) - (\mathbf{S} \otimes \mathbf{S})\mathbf{C}] = 0 . \quad (4.7)$$

In order to solve this equation for \mathbf{S} it is convenient to write \mathbf{M} in its spectral form

$$\mathbf{M} = \sum_{i=1}^m \lambda_i \mathbf{P}_i \otimes \mathbf{P}_i , \quad \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m > 0 , \quad \mathbf{P}_i \cdot \mathbf{P}_j = \delta_{ij} , \quad (4.8)$$

where λ_i are the positive ordered eigenvalues, \mathbf{P}_i are the associated orthonormal eigenvectors of \mathbf{M} and δ_{ij} is the generalized Kronecker delta. If \mathbf{S} is equal to one of the principle directions \mathbf{P}_i then \mathbf{A} vanishes and $\gamma = 0$, which means that \mathbf{R} is the exact rotation of the principle directions of \mathbf{M} . Furthermore, it can be shown that the maximum value γ_{\max} of γ occurs when \mathbf{S} is in the \mathbf{P}_1 - \mathbf{P}_m plane

$$\mathbf{S} = \cos\beta \mathbf{P}_m + \sin\beta \mathbf{P}_1, \quad (4.9)$$

so that (4.7) requires

$$\mathbf{A} \cdot (\mathbf{P}_1 \otimes \mathbf{P}_m) = \frac{\sin(2\beta)(\lambda_1 - \lambda_m)^2(\lambda_1 \sin^2\beta - \lambda_m \cos^2\beta)}{4(\lambda_1^2 \sin^2\beta + \lambda_m^2 \cos^2\beta)} = 0. \quad (4.10)$$

Thus, the values of β and γ_{\max} are given by

$$\beta = \tan^{-1}\left(\sqrt{\frac{\lambda_m}{\lambda_1}}\right), \quad \gamma_{\max} = \cos^{-1}\left[\frac{2\sqrt{\frac{\lambda_m}{\lambda_1}}}{1 + \frac{\lambda_m}{\lambda_1}}\right]. \quad (4.11)$$

It can easily be seen that this expression for γ_{\max} gives the maximum value of γ since it is based on the minimum value of the ratio λ_i/λ_1 . Moreover, this value of γ_{\max} determines the maximum error in the rotation of material line elements relative to that estimated by the rotation tensor \mathbf{R} . Figure 1 plots the value of γ_{\max} as a function of λ_m/λ_1 . In particular, it can be seen that if the distortional deformations are small with λ_m/λ_1 being close to unity then the maximum error made by the specification (4.1) is small. On the other hand, if the distortional deformations are large with small values of λ_m/λ_1 , then the angle γ_{\max} can be large.

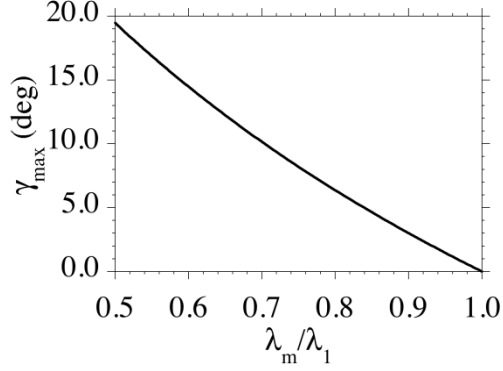


Fig. 1. Maximum angle of rotation γ_{\max} of material fibers relative to the rotation \mathbf{R} as a function of the stretch ratio λ_m/λ_1 .

5. Unphysical properties of the rotation tensor

The objective of this section is to discuss some unphysical properties of the rotation tensor $\mathbf{Q} = \bar{\mathbf{R}}$ determined in Section 3 using the least squares approximation with the constraint that \mathbf{F} be a rotation tensor. To this end, consider another set of vectors $\Delta\tilde{\mathbf{X}}_i$ which are defined by applying a pure rotation $\mathbf{\Lambda}$ to $\Delta\mathbf{X}_i$

$$\Delta\tilde{\mathbf{X}}_i = \mathbf{\Lambda}\Delta\mathbf{X}_i, \quad \mathbf{\Lambda}^T\mathbf{\Lambda} = \mathbf{I}, \quad \det(\mathbf{\Lambda}) = 1. \quad (5.1)$$

In general, the vectors $\Delta\mathbf{x}_i$ can experience rotation and stretching relative to $\Delta\mathbf{X}_i$ which is inhomogeneous. For this case the definitions of \mathbf{F} and \mathbf{Q} in (2.7), (2.8) and (4.1) are averages. Specifically, consider the simple case when $\{\Delta\mathbf{x}_i, \Delta\tilde{\mathbf{x}}_i\}$ are obtained by application of the *same* affine transformation \mathbf{F} to both $\Delta\mathbf{X}_i$ and $\Delta\tilde{\mathbf{X}}_i$

$$\Delta\mathbf{x}_i = \mathbf{F}\Delta\mathbf{X}_i, \quad \Delta\tilde{\mathbf{x}}_i = \mathbf{F}\Delta\tilde{\mathbf{X}}_i. \quad (5.2)$$

For this case, a body deforms from a fixed reference configuration by an affine deformation associated with \mathbf{F} and only the marked material line elements $\Delta\mathbf{X}_i$ on the body are changed to $\Delta\tilde{\mathbf{X}}_i$. Then, the estimate (3.5) of the rotation tensor \mathbf{Q} can be analyzed. To this end, it is

recalled that $\{\bar{\mathbf{F}}, \mathbf{H}\}$ associated with $\{\Delta\mathbf{X}_i, \Delta\mathbf{x}_i\}$ are given by (2.7). By analogy, $\{\tilde{\mathbf{F}}, \tilde{\mathbf{H}}\}$ associated with $\{\Delta\tilde{\mathbf{X}}_i, \Delta\tilde{\mathbf{x}}_i\}$ are defined by

$$\tilde{\mathbf{F}} = \sum_{i=1}^n \Delta\tilde{\mathbf{x}}_i \otimes \Delta\tilde{\mathbf{X}}_i = \tilde{\mathbf{F}}\tilde{\mathbf{H}} \quad , \quad \tilde{\mathbf{H}} = \sum_{i=1}^n \Delta\tilde{\mathbf{X}}_i \otimes \Delta\tilde{\mathbf{X}}_i = \Lambda\mathbf{H}\Lambda^T \quad . \quad (5.3)$$

Furthermore, applying the polar decomposition theorem to $\tilde{\mathbf{F}}$ yields

$$\tilde{\mathbf{F}} = \tilde{\mathbf{R}}\tilde{\mathbf{M}} \quad , \quad \tilde{\mathbf{R}}^T\tilde{\mathbf{R}} = \mathbf{I} \quad , \quad \tilde{\mathbf{M}}^T = \tilde{\mathbf{M}} \quad , \quad (5.4)$$

where $\tilde{\mathbf{R}}$ is a unique proper orthogonal rotation tensor and $\tilde{\mathbf{M}}$ is a unique positive definite stretch tensor. Thus, with the help of (3.5) it follows that $\mathbf{Q} = \bar{\mathbf{R}}$ for the unrotated orientation $\Delta\mathbf{X}_i$ associated with $\bar{\mathbf{F}}$, and $\mathbf{Q} = \tilde{\mathbf{R}}$ for the rotated orientation $\Delta\tilde{\mathbf{X}}_i$ associated with $\tilde{\mathbf{F}}$. Moreover, using (3.4), (5.3) and (5.4) it can be shown that

$$\bar{\mathbf{R}} = \mathbf{F}(\mathbf{H}\bar{\mathbf{M}}^{-1}) \quad , \quad \tilde{\mathbf{R}} = \tilde{\mathbf{F}}\tilde{\mathbf{H}}\tilde{\mathbf{M}}^{-1} = \mathbf{F}(\Lambda\mathbf{H}\Lambda^T\tilde{\mathbf{M}}^{-1}) \quad . \quad (5.5a,b)$$

Now, solving (5.5a) for \mathbf{F} and substituting the result into (5.5b) yields

$$\tilde{\mathbf{R}} = \bar{\mathbf{R}}(\bar{\mathbf{M}}\mathbf{H}^{-1}\Lambda\mathbf{H}\Lambda^T\tilde{\mathbf{M}}^{-1}) \quad . \quad (5.6)$$

To prove that $\tilde{\mathbf{R}}$ does not equal $\bar{\mathbf{R}}$ in general, assume that $\tilde{\mathbf{R}}$ equals $\bar{\mathbf{R}}$ so that (5.6) requires

$$\tilde{\mathbf{M}} = \bar{\mathbf{M}}\mathbf{H}^{-1}\Lambda\mathbf{H}\Lambda^T \quad . \quad (5.7)$$

Due to the symmetries of $\{\bar{\mathbf{M}}, \mathbf{H}, \tilde{\mathbf{M}}\}$ this condition yields the restriction

$$\bar{\mathbf{M}}\mathbf{H}^{-1}\Lambda\mathbf{H}\Lambda^T = \Lambda\mathbf{H}\Lambda^T\mathbf{H}^{-1}\bar{\mathbf{M}} \quad , \quad (5.8)$$

which is not valid for arbitrary rotation tensors Λ so $\tilde{\mathbf{R}}$ does not equal $\bar{\mathbf{R}}$ in general. This means that the estimation of the rotation tensor (3.5) exhibits an unphysical dependence on the orientation of the vectors $\Delta\mathbf{X}_i$ through the rotation tensor Λ . In the next section an example will be considered which shows that this rotation tensor also exhibits an unphysical dependence on the shape of the vectors $\Delta\mathbf{X}_i$ through the tensor \mathbf{H} .

In contrast, it follows from (2.7) and (5.3) that the tensors $\bar{\mathbf{F}}\mathbf{H}^{-1}$ and $\tilde{\mathbf{F}}\tilde{\mathbf{H}}^{-1}$ yield the correct affine transformation tensor \mathbf{F}

$$\mathbf{F} = \bar{\mathbf{F}}\mathbf{H}^{-1} = \tilde{\mathbf{F}}\tilde{\mathbf{H}}^{-1} , \quad (5.9)$$

so the alternative rotation tensor \mathbf{Q} proposed in (4.1), which equals the rotation tensor \mathbf{R} of \mathbf{F} , is unaffected by shape and orientation changes of the vectors $\Delta\mathbf{X}_i$.

6. A quantitative example

Consider the simple planar case with a triangular cluster of three points defined relative to the fixed rectangular Cartesian base vectors $\{\mathbf{e}_1, \mathbf{e}_2\}$ by

$$\mathbf{X}_1 = \mathbf{0} , \mathbf{X}_2 = L \mathbf{e}_1 , \mathbf{X}_3 = \alpha L \mathbf{e}_2 , \quad (6.1)$$

where L is a length measure and α controls the shape of the triangle (see Fig. 2). Next, consider the two-dimensional rotation tensor $\mathbf{\Lambda}$ defined by the angle θ

$$\mathbf{\Lambda} = (\cos\theta \mathbf{e}_1 + \sin\theta \mathbf{e}_2) \otimes \mathbf{e}_1 + (-\sin\theta \mathbf{e}_1 + \cos\theta \mathbf{e}_2) \otimes \mathbf{e}_2 , \quad (6.2)$$

with the rotated triangle in Fig. 2 defined by the points

$$\tilde{\mathbf{X}}_1 = \mathbf{0} , \tilde{\mathbf{X}}_2 = \mathbf{\Lambda}\mathbf{X}_2 , \tilde{\mathbf{X}}_3 = \mathbf{\Lambda}\mathbf{X}_3 . \quad (6.3)$$

Moreover, the rotated triangle is attached to a body which is distorted (deformed with no area change) by the homogeneous two-dimensional deformation gradient $\mathbf{F}\mathbf{F} = \mathbf{M}$

$$\mathbf{F} = \mathbf{M} = \lambda (\mathbf{e}_1 \otimes \mathbf{e}_1) + \frac{1}{\lambda} (\mathbf{e}_2 \otimes \mathbf{e}_2) , \quad \mathbf{R} = \mathbf{I} , \quad (6.4)$$

where λ is the stretch in the \mathbf{e}_1 direction and \mathbf{I} is the two-dimensional identity tensor. Using (5.3) and (5.4) the two-dimensional rotation tensor \mathbf{Q} is given by the two-dimensional rotation tensor $\tilde{\mathbf{R}}$ associated with the polar decomposition of the two-dimensional tensor $\tilde{\mathbf{F}}$ (5.4). In particular, \mathbf{Q} can be expressed in terms of the rotation angle ϕ in the form

$$\mathbf{Q} = \tilde{\mathbf{R}} = (\cos\phi \mathbf{e}_1 + \sin\phi \mathbf{e}_2) \otimes \mathbf{e}_1 + (-\sin\phi \mathbf{e}_1 + \cos\phi \mathbf{e}_2) \otimes \mathbf{e}_2 . \quad (6.5)$$

If $\lambda = 1$ with $\mathbf{M} = \mathbf{I}$ there is no deformation of the body and the rotation angle ϕ vanishes.

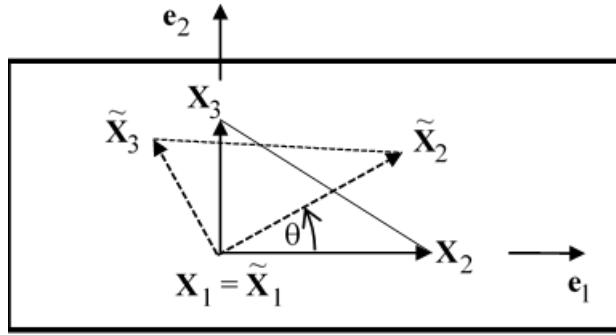


Fig. 2. Sketch of a body with the same triangular cluster of points oriented differently by the angle θ in the reference configuration.

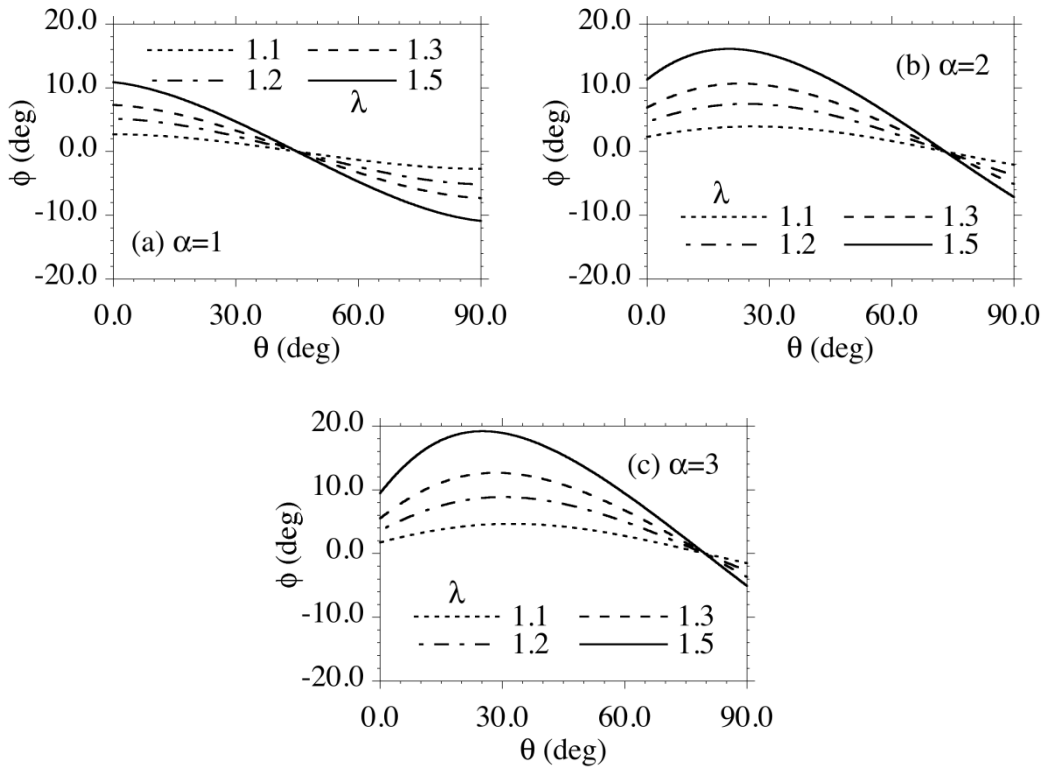


Fig. 3 Values of the rotation angle ϕ as a function of the orientation angle θ for different shapes α and stretches λ .

Figure 3 plots the values of the rotation angle ϕ as a function of the orientation angle θ for different values of the length ratio α and the stretch λ . In particular, it can be seen that ϕ exhibits an unphysical dependence on the shape $\{\alpha\}$ and orientation $\{\theta\}$ of the reference cluster with an error that increases with increasing deformation (stretch λ) and increasing

α . Moreover, for the deformation (6.4), the material line elements parallel to $\{\mathbf{e}_1, \mathbf{e}_2\}$ do not rotate. Consequently, any non-zero value of the rotation angle ϕ estimated by (6.5) represents an error. Also, using (5.3), (5.4) and (6.4) it follows that

$$\tilde{\mathbf{F}} = \tilde{\mathbf{R}}\tilde{\mathbf{M}} = \mathbf{M}\mathbf{\Lambda}\mathbf{H}\mathbf{\Lambda}^T . \quad (6.6)$$

Since the angle θ in $\mathbf{\Lambda}$ rotates the principle directions of \mathbf{H} , a value of θ exists for which the principle directions of $\mathbf{\Lambda}\mathbf{H}\mathbf{\Lambda}^T$ align with those of \mathbf{M} . For this value of θ the tensor (6.6) is symmetric with $\tilde{\mathbf{R}} = \mathbf{I}$ and with no error in ϕ for any value of λ that characterizes \mathbf{M} . These values of θ can be seen in Fig. 3 where the lines for different values of λ intersect at $\phi = 0$.

7. Discussion

The analysis in the previous sections shows that when the transformation of n vectors $\Delta\mathbf{X}_i$ into another set of n vectors $\Delta\mathbf{x}_i$ is approximated by a pure rotation, the least squares estimate of the rotation tensor \mathbf{Q} exhibits unphysical dependence on the shape and orientation of the reference data $\Delta\mathbf{X}_i$. In contrast, when the transformation is approximated by a general non-singular tensor \mathbf{F} , which includes deformation, the rotation tensor remains unaffected by shape and orientation changes of $\Delta\mathbf{X}_i$. Specifically, the average transformation tensor \mathbf{F} is defined by

$$\mathbf{F} = \left[\sum_{i=1}^n \Delta\mathbf{x}_i \otimes \Delta\mathbf{X}_i \right] \mathbf{H}^{-1} , \quad \mathbf{H} = \left[\sum_{j=1}^n \Delta\mathbf{X}_j \otimes \Delta\mathbf{X}_j \right]^{-1} , \quad (7.1)$$

where it is assumed that \mathbf{H} is non-singular. Further, assuming that the determinant of \mathbf{F} is positive, the polar decomposition theorem (2.8) is used to determine the unique proper orthogonal rotation tensor \mathbf{R} and the unique symmetric positive definite stretch tensor \mathbf{M} .

For biomechanical motion analysis, the rotation tensor \mathbf{R} can be used to estimate the pose of a bone segment in a structure of bone and soft tissue on which markers have been placed on the surface of the soft tissue. If this structure experiences homogeneous deformation and if the principle directions of \mathbf{M} remain constant with time then \mathbf{R} characterizes the rotation of the triad of material line elements that are parallel to these principle directions. Due to the homogeneity of the deformation this triad can be considered fixed (material) in the bone so \mathbf{R} predicts the bone orientation exactly.

However, if the deformation is inhomogeneous or if the principle directions of \mathbf{M} change with time then these principle directions do not remain material line elements of the bone so \mathbf{R} characterizes only an approximation of the bone orientation. The value γ_{\max} defined in (4.11) quantifies the maximum error in bone pose due to homogeneous deformations and it shows that the error increases with increasing distortional deformations and is small for small distortional deformations. In this regard, it is noted that if the cluster experiences an isotropic dilatation with all eigenvalues λ_i of \mathbf{M} in (4.8) being equal, then the deformation has no distortion with γ_{\max} in (4.11) vanishing. Consequently, for small distortional deformations, \mathbf{R} can be used with confidence to estimate the bone pose.

Since the tissue is typically much softer than the underlying bone, the deformation of the tissue-bone structure is almost always inhomogeneous so that an average \mathbf{F} cannot be expected to accurately estimate the bone pose unless the deformations remain small. Recently (Solav et al., 2014, 2015) Triangular Cosserat Point Elements (TCPEs) have been developed to analyze the cluster of markers. All combinations of three markers are used to define a group of TCPEs which are based on general homogeneous deformations of triangles. For cases when the actual motion of the bone segment is known, it has been shown that different subsets of TCPEs more accurately characterize bone position and orientation than estimations based on the entire group of TCPEs (Solav et al., 2015). Moreover, physical measures based on deformations of each TCPE and on relative translations and rotations between pairs of TCPEs are being used to quantify the characteristics of the most accurate TCPEs for the estimation of bone position and orientation (Solav et al., 2015). Since the TCPE method is based on a number of TCPEs it can also be used to analyze the inhomogeneity in a deformation field which can reveal relative motion between different segments of the body. More specifically, the TCPE approach adds a vector normal to the triangle in order to define a non-singular \mathbf{F} for full three-dimensional homogeneous deformations.

Now that the mathematical and physical background of the estimates of rotation have been presented it is possible to discuss the relationship of this work with previous work reported in the literature. All works (Schonemann, 1966; Wahba, 1966; Spoor and Veldpaus, 1980; Arun et al., 1987; Veldpaus et al., 1988; Besl and McKay, 1992;

Soderkvist and Wedin, 1993; Challis, 1995) which use the rigid body approximation based on the least squares method to determine the rotation tensor \mathbf{Q} exhibit the unphysical properties discussed above. Consequently, here attention will be limited to works that use an affine transformation approximation which includes deformations of the data. Hurley and Cattell (1962) developed a tensor similar to the transpose of \mathbf{F} in (2.7) for application in behavioral science. Although they discussed unrotated data, which suggests that they are attempting to find an average rotation tensor, their statement that they normalize the columns of this tensor is not clear enough to determine if their method is the same as using the polar decomposition theorem to determine a rotation tensor \mathbf{Q} equal to the rotation tensor \mathbf{R} in the polar decomposition theorem (2.8). Lew and Lewis (1977) developed an affine approximation for anthropometric scaling of rigid body motion models adapted to different sized humans. Sommer et al. (1982) developed the transpose of the average deformation tensor \mathbf{F} in (2.7) and proposed an averaging procedure on the stretch tensor in the polar decomposition theorem (2.8) for different specimens to develop a method for osteometric scaling and normative modeling of skeletal segments. Moreover, it is noted that these authors (Lew and Lewis, 1977; Sommer et al., 1982) did not apply their work to the analysis of the underlying bone pose from a cluster of markers. Dumas and Cheze (2009) compared different methods for bone pose estimation, one of which used the rotation tensor of the deformation gradient developed by Sommer et al. (1982). This estimate is essentially identical to the alternative rotation tensor discussed here in Section 4. Ball and Pierrynowski (1998) adopted the affine method of stretching and rotating bodies for animation from the field of computer science to develop a pliant surface model which approximates the motion of the cluster as a homogeneous deformation. Specifically, they proposed a form for \mathbf{F} with a rotation tensor multiplied by a deformation tensor. However, their deformation tensor was based on specific assumptions about stretching and shearing of the cluster, it exhibits order dependence on these deformation operations and is not a symmetric stretch tensor. Consequently, their rotation tensor is different from the rotation tensor \mathbf{R} of \mathbf{F} defined by the polar decomposition theorem (2.8) and used here.

Sommer et al. (1982) considered a rotation similar to $\mathbf{\Lambda}$ in (5.3) for the purpose of showing that their transformation tensor is unaffected by mirror image transformations. However, they did not recognize the stronger implications of using an average deformation

gradient \mathbf{F} to obtain an average rotation tensor \mathbf{R} which is unaffected by shape and orientation changes of points in the reference configuration.

The main new aspect of the work in this paper is to prove that when the transformation of the data set \mathbf{X}_i into \mathbf{x}_i is approximated by a translation and rotation, then the rotation tensor \mathbf{Q} obtained by least squares optimization exhibits an unphysical dependence on the orientation and shape of the reference cluster \mathbf{X}_i , as shown in the example in Section 6. Also, the value γ_{\max} in (4.11) is a new measure which gives an upper bound for the error in estimating the orientation of the underlying bone pose in a bone-tissue structure experiencing homogeneous deformations.

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