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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 $\mathbf{X}_i$ $(i = 1, 2,\ldots,n)$ 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.

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 & Cattell, 1962; Schonemann, 1966); satellite attitude estimation (Wahba, 1966); registration and motion of 3-D shapes (Arun, Huang, & Blostein, 1987; Besl & McKay, 1992; Laub & Shiflett, 1982); anthropometric scaling (Lew & Lewis, 1977; Sommer, Miller, & Pijanowski, 1982); and biomechanical motion analysis (Ball & Pierrynowski, 1998; Cappozzo, Catani, Leardini, Benedetti, & Della Croce, 1996; Cappozzo, Della Croce, Leardini, & Chiari, 2005; Challis, 1995; Dumas & Cheze, 2009; Soderkvist & Wedin, 1993; Spoor & Veldpaus, 1980; Veldpaus, Woltring, & Dortmains, 1988), 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 (Dumas & Cheze, 2009; Leardini, Chiari, Della Croce, & Cappozzo, 2005; Peters, Galna, Sangeux, Morris, & Baker, 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 $\mathbf{X}_i$ $(i = 1, 2,\ldots, n)$ 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).

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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., Arun et al., 1987; Besl & McKay, 1992; Challis, 1995; Schonemann, 1966; Soderkvist & Wedin, 1993; Spoor & Veldpaus, 1980; Veldpaus et al., 1988; Wahba, 1966) 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 $\{\bar{\mathbf{X}}, \bar{\mathbf{x}}\}$ of $\{\mathbf{X}_i, \mathbf{x}_i\}$ by the expressions

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

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

$$\mathbf{X}_i = \bar{\mathbf{X}} + \Delta\mathbf{X}_i, \; \mathbf{x}_i = \bar{\mathbf{x}} + \Delta\mathbf{x}_i. \tag{2.2}$$

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

$$\mathbf{x}_i^* = \bar{\mathbf{X}} + \mathbf{t} + \mathbf{F}\Delta\mathbf{X}_i, \tag{2.3}$$

where $\mathbf{t}$ is the approximate translation vector of $\bar{\mathbf{X}}$ 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)

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

where $(\cdot)$ 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

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

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

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

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

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

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 $\Delta\mathbf{X}_i$.