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APPENDIX

Transforming *Surface₂* to *Surface₁*

Our matrix conventions for transforming surface points and surface normals between two surfaces are described below. The conventions are the standard nomenclature used in the field of geometric morphometrics [1].

Let

$$d_2 = [\, x \quad y \quad z \quad 1 \,]$$

be a set of points on *Surface*$_2$ and

$$n_2 = [\, nx \quad ny \quad nz \quad 1 \,]$$

be a set of surface normals on *Surface*$_2$. The first three terms in each vector represent magnitudes for the three directions (*x,y,z*). The fourth term is a scaling terms. Because we perform no scaling in our optimization, the fourth term is set to a value of 1.

The translations and rotations to transform the data from *Surface*$_2$ to *Surface*$_1$ are

$$\boldsymbol{T} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ T_x & T_y & T_z & 1 \end{bmatrix}$$

$$\boldsymbol{R_x} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & cos\theta_x & sin\theta_x & 0 \\ 0 & -sin\theta_x & cos\theta_x & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{R_y} = \begin{bmatrix} cos\theta_y & 0 & -sin\theta_y & 0 \\ 0 & 1 & 0 & 0 \\ sin\theta_y & 0 & cos\theta_y & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{R_z} = \begin{bmatrix} cos\theta_z & sin\theta_z & 0 & 0 \\ -sin\theta_z & cos\theta_z & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where T_x, T_y, and T_z are translations along the *x, y,* and *z* axes, and θ_x, θ_y, and θ_z are rotations about the *x*, *y*, and *z* axes. The goal of the alignment algorithm described below is to determine T_x, T_y, T_z, θ_x, θ_y, and θ_z.

During the optimization process, T_x, T_y, T_z, θ_x, θ_y, and θ_z are real numbers (after an initial guess of [0 0 0 0 0 0], they are calculated in each iteration) . The transformation matrix to transform *Surface*$_2$ to *Surface*$_1$ is

$$\boldsymbol{M_{2to1} = T\, R_x\, R_y\, R_z}$$

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Thus the operation to transform the set of points on *Surface₂* to *Surface₁* is

$$d_1 = d_2\, \boldsymbol{M_{2to1}}$$

To transform the data back to *Surface₂* the inverse of the transformation matrix is used

$$\boldsymbol{M_{1to2}} = \boldsymbol{M_{2to1}^{-1}}$$

$$d_2 = d_1 \boldsymbol{M_{1to2}}$$

Surface normals are not transformed the same as surface points. To transform the surface normal vector, the inverse transpose of the transformation matrix is used [2]

$$\boldsymbol{N_{2to1}} = [\boldsymbol{M_{2to1}^{-1}}]^{\boldsymbol{T}}$$

$$n_1 = n_2 \boldsymbol{N_{2to1}}$$

To transform the surface normal vector back to *Surface₂* the inverse of the transformation matrix is used

$$\boldsymbol{N_{1to2}} = \boldsymbol{N_{2to1}^{-1}}$$

$$n_2 = n_1 \boldsymbol{N_{1to2}}$$

Alignment Algorithm

1. Fit *Dataset #1* (the normally-used socket) with a tensor product B-spline to create *Surface₁*.

A tensor product B-spline surface is the result of a tensor product of two B-spline curves. The surface is defined by a rectilinear grid of control points. See Farin and Hansford [3].

2. Fit *Dataset #2* (the test socket) with a tensor product B-spline to create *Surface₂*.
3. Sample *Surface₁* at an evenly-spaced [θ,z] grid, defining the new set of points as

$$d_1^A = [x \;\; y \;\; z \;\; 1\,]$$

Calculate the surface normals at each of these points and define them as

$$n_1^A = [\,n_x \;\; n_y \;\; n_z \;\; 1\,]$$

Note that in the optimization process described below, the normal vectors need to be unit vectors.

4. Input optimization parameters

Provide initial guess of T_x, T_y, T_z, θ_x, θ_y, and θ_z. Use [0 0 0 0 0 0]. Note that to use this initial guess, the two datasets need to be reasonably well aligned at the outset. In the present study we

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accomplish this alignment by taking care when setting up the sockets in the digitizer so that the *z*-axis is well aligned with the centroids of the socket cross-sections, and the stylus arm at the outset of digitizing is at a tangential position corresponding to the center of the patellar tendon bar.

a. Set limits on translation and rotation. In the present study we used translation limits of -40 mm to +40 mm, and rotation limits of -45° to 45°.
b. Specify use of the active set algorithm. "Active set" is a Matlab term indicating that the gradient of the objective function is not to be provided by the user.
c. Set termination tolerance on the solution. In the present study we used a value of 10^{-6}.

5. Run the optimization routine with a *RadialWeight* of 1.0 and a *NormalWeight* of 0.0 to completion:

In Matlab, use *fmincon* with the objective function *f* described below in section 5.e to determine T_x, T_y, T_z, θ_x, θ_y, and θ_z.

Optimization loop

a. Transform $Surface_1$ to $Surface_2$ using the inverse of the alignment transformation matrix (either the initial guess or that resulting from the prior iteration)

$$d_2^A = d_1^A \boldsymbol{M_{1to2}}$$

$$n_2^A = n_1^A \boldsymbol{N_{1to2}}$$

b. Sample $Surface_2$ at the same [θ,*z*] locations as the transformed data from $Surface_1$. The set of points is d_2^B. The *z* values are the *z* values of d_2^A. The θ values are the arctangents values (*atan(y/x)*) of d_2^A. Also calculate the normals at each point. This set of normals is n_2^B. If there are no corresponding points on the two surfaces because one surface extends more proximally or distally than the other, then those points are dropped from the analysis for the iteration.
c. Calculate the mean radial error

$$r_2^A = \sqrt{d_2^A x^2 + d_2^A y^2 + d_2^A z^2}$$

$$r_2^B = \sqrt{d_2^B x^2 + d_2^B y^2 + d_2^B z^2}$$

$$MnRadialError = mean(r_2^B - r_2^A)$$

d. Calculate the mean hyperbolic arctangent of the dot product of the normals, which is the Normal Similarity term used in the objective function,

$$NormalSimilarity = mean(\tanh^{-1}(n_2^A . n_2^B - 10^{-7}))$$

The dot product of two parallel unit vectors is equal to 1.

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10^{-7} is subtracted from the dot product of the normals because when the normals are parallel to each other the dot product is 1. The hyperbolic arc tangent of 1 is infinity which distorts the analysis and thus needs to be avoided.

e. Calculate the value of the objective function

$$f = RadialWeight \times MnRadialError - NormalWeight \times NormalSimilarity$$

Because the objective function is minimized within the optimization routine, the second term which maximizes shape similarity is subtracted from the first.

In this optimization routine, a *RadialWeight* of 1.0 and a *NormalWeight* of 0.0 are used (as indicated above), and the translational and rotational transformation matrices calculated. They are then used as an initial guess in the second optimization routine, step 6.

6. Run second optimization routine to completion

Repeat the optimization using the initial guess from step 5 and a *RadialWeight* of 0.8 and *NormalWeight* of 0.2.

The T_x, T_y, T_z, θ_x, θ_y, and θ_z values calculated from this optimization are the settings used in the transformation matrices to align $Surface_1$ and $Surface_2$.

When a collection of surfaces are compared to a reference surface (e.g., the three test sockets to the original socket in the present study), the bounds of *z* that include all surfaces are determined, and only data within those bounds are used in analysis.

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