Morphometric mappings between surfaces embedded in 3D.

Problems in which an unparametrized surface is given and a parameterized surface is desired arise in many situations. For example, often you have two images of analogous (homologous) objects and a specific matching between the points on the two images is desired. Another example occurs with agents moving across a terrain with desired distance between them. In this situation, the registration problem gives the trajectories of the agents given the shape of the occupied terrain. In this paper, we work out a formalism to describe shape changes between surfaces in $\mathbb{R}^3$ and a solution to the registration problem for time evolving surfaces.

I. 3D FORMALISM

We want to extend quasi-conformal mappings between planar domains to mappings between closed surfaces embedded in 3D.

Assume we have a surface $\mathbf{X}_0(\mathbf{u}) : \Omega \to \mathbb{R}^3$, were $(u^1, u^2) \equiv \mathbf{u} \in \Omega \subset \mathbb{R}^2$, and another surface $\mathbf{X}(\mathbf{y}) : \Omega' \to \mathbb{R}^3$. A map between these surfaces, a registration, would be given by the functions $\mathbf{y}(\mathbf{u}) : \Omega \to \Omega'$, where the bold face notation represents vectors in $\mathbb{R}^3$ if the letter is capitalized and $\mathbb{R}^2$ otherwise.

There are many possible smooth maps that can connect the two surfaces, which are in one-to-one correspondence with the diffeomorphisms of $\mathbf{X}_0(\mathbf{u})$. We can distinguish between these mappings – up to conformal isometries – by considering the eccentricity of ellipses on $\mathbf{X}(\mathbf{y})$ which started as infinitesimal circles on $\mathbf{X}_0(\mathbf{u})$, as in the theory of quasi-conformal mappings. More generally, we want to minimize some generalized notion of distance between the two surfaces in order to determine the registration. Following [1], we will consider using the elastic distortion as a notion of distance between surface. The elastic distortion can be decomposed into expansion, shearing and twisting which we calculate next.

Firstly, we define the induced metric on $\mathbf{X}_0$, which gives distances and angles between curves on the surface, as

$$\bar{g}_{ij}(\mathbf{u}) \equiv \frac{\partial \mathbf{X}_0}{\partial u^i} \cdot \frac{\partial \mathbf{X}_0}{\partial u^j} \equiv \partial_i \mathbf{X}_0 \cdot \partial_j \mathbf{X}_0. \tag{1}$$

And similarly for $\mathbf{X}(\mathbf{y})$ we can find $g_{ij}(\mathbf{y})$. Second, for a given registration $\mathbf{y}(\mathbf{u})$, we can relate the two metrics using the deformation vector $\mathbf{Y}(\mathbf{u})$ as

$$\begin{aligned}
&\mathbf{Y}(\mathbf{u}) \equiv \mathbf{X}(\mathbf{y}(\mathbf{u})) - \mathbf{X}_0(\mathbf{u}) \quad \Longrightarrow \\
&g_{ij}(\mathbf{u}) = \bar{g}_{ij} + \partial_i \mathbf{X}_0 \cdot \partial_j \mathbf{Y} + \partial_i \mathbf{Y} \cdot \partial_i \mathbf{X}_0 + \partial_i \mathbf{Y} \cdot \partial_j \mathbf{Y}. \qquad (2)
\end{aligned}$$

Note that the metric $g_{ij}(\mathbf{u})$ is written with respect to the $\mathbf{u}-$coordinates since the registration allows us to write the two surfaces with respect to a common coordinate neighborhood $\Omega \subset \mathbb{R}^2$. Now we're in a position to start calculating the eccentricity, or shear, of the transformation. We will represent a circle in the tangent plane of the surface at an arbitrary point using an orthonormal field of vectors tangent to the surface $\bar{\mathbf{e}}^i_a, a = 1, 2$, where i indexes the components of the vectors in the $\mathbf{u}$-coordinate frame and a indexes the orthonormal vector. By orthonormality and completeness, we have that

$$\bar{g}_{ij}\ \bar{\mathbf{e}}^i_a\ \bar{\mathbf{e}}^j_b = \delta_{ab} \text{ and } \bar{\mathbf{e}}^i_a\ \bar{\mathbf{e}}^j_b\ \delta^{ab} = \bar{g}^{ij}. \qquad (3)$$

A circle in the tangent space of a point is traced out by $\mathbf{v}^i(\theta) = \cos(\theta)\ \bar{\mathbf{e}}^i_1 + \sin(\theta)\ \bar{\mathbf{e}}^i_2 \equiv v^a\ \bar{\mathbf{e}}^i_a,\ \theta \in [0, 2\pi)$. Since by construction we are using the same coordinates on both surface, the deformed circle on the surface $\mathbf{X}$ is represented by the same coordinates $\mathbf{v}^i(\theta)$. However, the length squared of the vector in the deformed configuration will then be given by $L^2[v^i(\theta)] = g_{ij}\ \mathbf{v}^i\ \mathbf{v}^j$, while the square of the eccentricity, $e^2_{\mathbf{Y}}$, is given by

$$e^2_{\mathbf{Y}} \equiv \frac{\sup\limits_{\theta}\ [\ L^2(\theta)]}{\inf\limits_{\theta}\ [\ L^2(\theta)]}. \qquad (4)$$

More explicitly, we can write the length squared as

$$L^2[\mathbf{v}^i(\theta)] = v^a\ v^b\ L_{ab}. \qquad \text{where} \qquad L_{ab} \equiv g_{ij}\ \bar{\mathbf{e}}^i_a\ \bar{\mathbf{e}}^j_b \qquad (5)$$

Now we see that $e^2_{\mathbf{Y}}$ is the ratio of the largest eigenvalue of L_{ab} to the smallest, which can be calculated by knowing the trace of both L_{ab} and its square L^2_{ab}. After some manipulations and using Eq. (3) we get

$$e^2_{\mathbf{Y}} = \frac{1 + d_{\mathbf{Y}}}{1 - d_{\mathbf{Y}}} \geq 1 \qquad \text{where} \qquad d_{\mathbf{Y}} \equiv \sqrt{2\frac{Tr[L^2]}{Tr[L]^2} - 1} = \sqrt{2\frac{g_{ij}g_{k\ell}\ \bar{g}^{ik}\bar{g}^{j\ell}}{g_{ij}g_{k\ell}\ \bar{g}^{ij}\bar{g}^{k\ell}} - 1}. \qquad (6)$$

We have used the fact that $Tr(L) = g_{ij}\bar{g}^{ij}$ and $Tr(L^2) = g_{ij}g_{k\ell}\ \bar{g}^{ik}\bar{g}^{j\ell}$. We may also find the dilation of the circle as $\Omega_{\mathbf{Y}} = \sqrt{\det L}$, where $\det L = (g_{ij}\ g_{k\ell}\ \bar{g}^{ij}\ \bar{g}^{k\ell} - g_{ij}g_{k\ell}\ \bar{g}^{ik}\bar{g}^{j\ell})/2$. The direction of the largest eigenvalue of L_{ab}, given by the angle $\theta_{\mathbf{Y}}(\mathbf{u})$, gives the orientation of the major axis of the ellipse relative to the chosen orthonormal frame $\bar{\mathbf{e}}_a^i$.

Now, in order to solve for the optimal registration between the two surfaces we will consider the following cost function (also referred to as the elastic distance, in analogy to the elastic energy in physics) which gives a generalized notion of distance between two surfaces

$$dist\left[\mathbf{X_0}(\mathbf{u}), \mathbf{X}(\mathbf{y}(\mathbf{u}))\right] = \int dA_{\mathbf{X_0}} \left[a \ (\Omega_{\mathbf{Y}} - 1)^2 + b \ (e_{\mathbf{Y}} - 1)^2 + c \ (\boldsymbol{\nabla}_{\mathbf{X_0}} \Omega_{\mathbf{Y}})^2 + d \ (\boldsymbol{\nabla}_{\mathbf{X_0}} e_{\mathbf{Y}})^2 + \cdots \right]. \quad (7)$$

A term depending on $\theta_{\mathbf{Y}}$ could be added if an implicit background unit vector field is defined on the surface, which would provide the reference angle. For example, a frame of reference in which to define the angle might be given by the principle directions. Note that the cost function defined here is not a real distance since it is not symmetric in its arguments and could be zero when $\mathbf{X}$ is an isometric deformation of $\mathbf{X}_0$. If a symmetric function is desired, we can symmetrize this functional by either taking the average of the two directed distances or the maximum of the two. The second possible issue is solved below by adding terms that include extrinsic differences between the surfaces, for example changes in the surface normals. Finally, we might add to this terms biasing registrations that maximize correlation between growth and some field on the surface. If $a, c, d = 0$, then this cost function favors conformal (or Teichmüller) maps. If $b, c, d = 0$, then intuitively speaking, the cost function favors growth with the least amount of added material at each point.

In the case where we have infinitesimal changes in the surface with time, for example in a growing organism, the notion of a distance between surfaces will generalize to a Riemannian metric on the space of shapes. Next, we turn to the description of dynamically growing shapes.

II. GROWTH REPRESENTATIONS

The change in the metric from $\bar{g}_{ij}$ to g_{ij} can be represented in several different forms, for example, using expansion, shear and twist. In a coordinate system where $\bar{g}_{ij}$ is locally flat, the change can be represented as a combination of areal strain, shear and rotation. Since the initial metric is positive definite and symmetric at every point on the surface, it can be written as $\bar{g}_{ij} = \Lambda^T \ \Lambda$. Here $\Lambda(\mathbf{u})$, at each point $\mathbf{u}$, could be thought of as a coordinate transformation between the locally flat coordinate system $\tilde{u}^i$ and an arbitrary coordinate system u^i. Combining this with the deformations we can write the new metric as

$$g_{ij} = \Omega \ \Lambda^T \ R^T E \ R \ \Lambda, \qquad E \equiv \begin{pmatrix} 1+e & 0 \\ 0 & \frac{1}{1+e} \end{pmatrix} \quad (8)$$

where Ω is the stretching factor, e is the eccentricity and R is a rotation matrix giving the direction of the major axis.

We are also interested in the instantaneous deformation, or time derivative of the metric as we will see in the next section. Taking the time derivative of Eq. (8), we get

$$\dot{g}_{ij} = \frac{\dot{\Omega}}{\Omega}\, g_{ij} + \frac{\dot{e}}{1+e}\Omega\Lambda^T R^T E\sigma_Z R\Lambda + \Omega\Lambda^T \left[\dot{R}^T R, R^T E R\right] \Lambda.$$

This equation gives us the instantaneous change in the metric as three contributions; areal, shear and rotational strains. The dot over the function denotes time derivatives, σ_Z is a Pauli matrix and $[A, B] \equiv AB - BA$ denotes a commutator. We imagine that we already have $\dot{g}_{ij}$ after solving the registration problem.

Next we show how to obtain the deformation functions from the time derivative of the metric. In the previous section we saw how to find e, Ω and the rotation angle θ, here we will show how to obtain the infinitesimal version of these relations. The isotropic expansion factor can be found as

$$\frac{1}{2} Tr \left[g^{ij}\dot{g}_{ij}\right]^2 = \left(\frac{\dot{\Omega}}{\Omega}\right)^2 . \tag{9}$$

The rate of change in eccentricity can be expressed through the relation

$$\begin{aligned} \frac{1}{2} Tr \left[(g^{ij}\{\dot{g}_{ij}\})^2\right] &= \left(\frac{\dot{e}}{1+e}\right)^2 + Tr\left[\left(R\,\dot{R}^T\right)^2 - R\,\dot{R}^T E^{-1} R\,\dot{R}^T\,E\right] \\ &= \left(\frac{\dot{e}}{1+e}\right)^2 + \frac{\left[2+e(\mathbf{u},t)\right]^2\; e^2(\mathbf{u},t)\;\dot{\theta}_{\mathbf{Y}}(\mathbf{u},t)}{\left[1+e(\mathbf{u},t)\right]^2} \end{aligned} \tag{10}$$

where $\{\dot{g}_{ij}\}$ is the traceless part of the metric change and $\theta_{\mathbf{Y}}$ is the rotation angle of the matrix R such that $R_{21} = \sin\theta_{\mathbf{Y}}$. Note that the trace on the right hand side above is zero at $t = 0$, since $E(t = 0) = \mathbb{I}_2$. Since by definition we have $g_{ij}(t = 0) = \bar{g}_{ij}$, eccentricity will satisfy

$$e(\Delta t) \approx \dot{e}(t=0)\;\Delta t = \frac{1}{2} Tr \left[(\bar{g}^{ij}\{\dot{g}_{ij}(t=0)\})^2\right]\;\Delta t. \tag{11}$$

III. DYNAMICS

Assume we are given a series of *unparameterized* surfaces, $\mathbf{S}(t)$, labeled by time. We want to find a *parameterized* flow of surfaces $\mathbf{X(t)}$, a registration, that describes this evolution. Starting with unparameterized surfaces presents a problem to the dynamic case since in an infinitesimal time interval dt, the deformation (reparameterization) can be finite. This is true because the same shape $\mathbf{S}(t)$ can correspond to different functions $\mathbf{X(t)}$ by changing the registration. We would still like to take advantage of the fact that during the interval $(t, t + dt)$, the surface deformed only

slightly. In other words, it will be difficult to describe the change by giving the dependence of the time derivative of the metric, $\partial_t g_{ij}(t)$, on local functions.
We can get over this problem in several ways. We can get rid of rotations by first finding the best fitting ellipsoid for each surface then aligning the directions of the ellipsoid axes. Similarly translations can be taken care of by finding the center of "mass" for each surface and aligning them. If there are landmarks on the surfaces, we can also use those to align the surface, by bringing the landmarks close to each other.

Assuming proper alignment, we can now describe the evolution of the shapes by a differentiable function $\mathbf{X}(\mathbf{y}(\mathbf{u},t),t)$, where $\mathbf{y}(\mathbf{u},t)$ is the unknown registration. Proper alignment implies that the function $\mathbf{y}(\mathbf{u},t)$ is differentiable with respect to time or that changes in $\mathbf{y}(\mathbf{u},t)$ will be infinitesimal for infinitesimal changes in time. This fact implies that $\partial_t \mathbf{y}(\mathbf{u},t)$ is an infinitesimal diffeomorphism (change of coordinates) which is in one-to-one correspondence with a vector field in the tangent space of the surface $\mathbf{X}(\mathbf{y}(\mathbf{u},t),t)$. The fact that we are solving for a vector tangent to the surface will become clear in the section describing the implementation of the algorithm (Sec. IV).

In order to solve the registration problem for the infinitesimal or dynamic case, we will have to introduce a notion of distance between two surfaces as done before in the finite case. However, in the present situation the distance turns into a Riemannian metric defined on the space of all surfaces embedded in $\mathbb{R}^3$. A Riemannian metric is a bilinear form on the tangent space of the manifold. Curves in this manifolds are one parameter family of surfaces $\mathbf{X}(\mathbf{u},\lambda)$, parameterized by λ. The tangent space at a given surface $\mathbf{X}_0(\mathbf{u})$ is in correspondence to the set of all curves $\mathbf{X}(\mathbf{u},\lambda)$ passing through it at $\lambda = 0$ with tangents given by $\mathbf{V}(\mathbf{u},t) = \dot{\mathbf{X}}(\mathbf{u},t)$. Note here that when say curves or tangents, we are referring to the manifold of all parameterized surfaces, not to curves or vectors tangent to a single surface. When calculating the length of the path $\mathbf{X}(\mathbf{u},\lambda)$, $\lambda \in [0,1]$, we use chose the elastic metric,

$$\langle \mathbf{V}_1, \mathbf{V}_2 \rangle = \int dA \left(A\, Tr\left[\{g^{-1}\dot{g}_1\} \{g^{-1}\dot{g}_2\} \right] + B\, Tr\left[g^{-1}\dot{g}_1 \right]\ Tr\left[g^{-1}\dot{g}_2 \right] + C\, \dot{\mathbf{n}}_1 \cdot \dot{\mathbf{n}}_2 \right), \tag{12}$$

where $\mathbf{n}_1(t)$ is the normal vector of the first family of surfaces and $g_1(t)$ is the corresponding induced metric. In the first two terms in this metric A, B correspond physically to The shear and bulk moduli respectively. The last term in this equation which penalizes bending can be used to distinguish between isometries.

In the next section we will show how to solve the registration problem by requiring the length of the path $\mathbf{X}(\mathbf{u},t)$ to be as small as possible.

IV. THE REGISTRATION ALGORITHM

We start by describing an algorithm for numerically calculating the infinitesimal length of a tangent vector $\mathbf{V}(\mathbf{u}, t)$ in the manifold of parameterized surface. The "length" here can also be thought of as an elastic energy.

We calculated this length approximately by triangulating the surface and calculating the contribution from each triangle separately. We start with triangles on the undeformed surface $\mathbf{X}(t)$ and deform them to the be on the surface $\mathbf{X}(t + dt) = \mathbf{X}(t) + \mathbf{V}(t)\ dt$. Each triangle has three vertices with positions $\bar{\mathbf{P}}_0, \bar{\mathbf{P}}_1$ and $\bar{\mathbf{P}}_2$. In order to specify a coordinate system on the triangles, we define the vectors $\bar{\mathbf{v}}_a = \bar{\mathbf{P}}_0 - \bar{\mathbf{P}}_a,\ a = 1, 2$. We can introduce the coordinate system $(\bar{u}^1, \bar{u}^2) \in [0, 1]^2$, where the position of a point on the triangle is given by $\bar{\mathbf{P}} = \bar{\mathbf{P}}_0 + \bar{u}^a\ \bar{\mathbf{v}}_a$. We can find the metric and normal vector in this coordinate system as

$$\bar{g}_{ab} = \bar{\mathbf{v}}_a \cdot \bar{\mathbf{v}}_b = \begin{pmatrix} \bar{\mathbf{v}}_1 \cdot \bar{\mathbf{v}}_1 & \bar{\mathbf{v}}_1 \cdot \bar{\mathbf{v}}_2 \\ \bar{\mathbf{v}}_1 \cdot \bar{\mathbf{v}}_2 & \bar{\mathbf{v}}_2 \cdot \bar{\mathbf{v}}_2 \end{pmatrix}, \qquad \hat{\bar{n}} = \frac{\bar{\mathbf{v}}_1 \times \bar{\mathbf{v}}_2}{\sqrt{\bar{g}}} \tag{13}$$

Now we want to find the deformation in the metric, $\dot{g}_{ab}$ given the deformations of the vertices $\delta\bar{\mathbf{P}}$, keeping in mind that the final positions $\bar{\mathbf{P}}$ will lie on the given deformed surface. We may decompose the deformation into parts tangent to the surface $\mathbf{X})(t)$ and parts normal to it, $\delta\bar{\mathbf{P}} = \delta\bar{\mathbf{P}}_{||} + \delta\bar{\mathbf{P}}_n$. We are trying to find the deformation that minimizes the given elastic metric. Note that only the tangent displacement is unknown here and is to be minimized over. The normal displacements cannot be changed during optimization since they define the unparametrized surface and not the registration (parameterization). This is consistent with what we noted in Sec. (I), that the registration problem is equivalent to finding the diffeomorphism $\mathbf{y}(\mathbf{u})$. In the infinitesimal case, a diffeomorphism is a displacement in the tangent space only.

Now we are in a position to find the change in the metric. Namely, $\dot{g}_{ab} = \bar{\mathbf{v}}_a \cdot \delta\mathbf{v}_b + \bar{\mathbf{v}}_b \cdot \delta\mathbf{v}_a$. With that, we have all the ingredients needed to calculate the elastic metric contribution from the triangle. We can then sum the result for each triangle and multiply by the individual areas $dA = \sqrt{\bar{g}}$.

The algorithm is as follows

- Start with two shapes infinitesimally deformed from each other.
- Triangulate the initial surface.
- For each vertex find an orthonormal frame with a normal to the surface and two tangents.

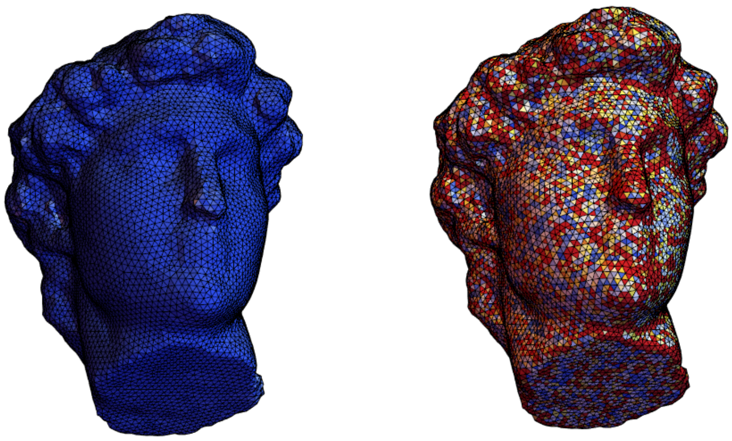

Figure 1: Shows and output of the minimization procedure described above. The figure on the right shows the cost of morphing the surface for each triangle from random initial tangent displacement. The figure on the left shows the results after minimization normalized to the same value. Here red represents 1 and blue zero and the data is normalized to the mean value in the initial displacements, before minimization.

- For each vertex project out a ray normal to the surface and find where it intersects the deformed surface. record this as the normal displacement.
- Initialize the tangent displacements.
- Define the discretized version of the elastic metric and calculate the gradient and Hessian with respect to tangent displacements as sketched above.
- Use Newton-conjugate-gradient algorithm in Python (Scipy library) to minimize the elastic metric with respect to tangent displacements.
- Add the resultant displacements to the initial vertices. Each triangle can be color coded according to its contribution to the elastic metric or according to shear, dilation, etc., see Figs. (1, 2).

V. CHARACTERIZING THE ALGORITHM

The current algorithm finds the registration that minimizes the elastic deformations. Roughly speaking the two surfaces are interpolated with a deformation that is nearly isometric, one that changes the metric as little as possible. For example, if the two surface are planar, the optimal

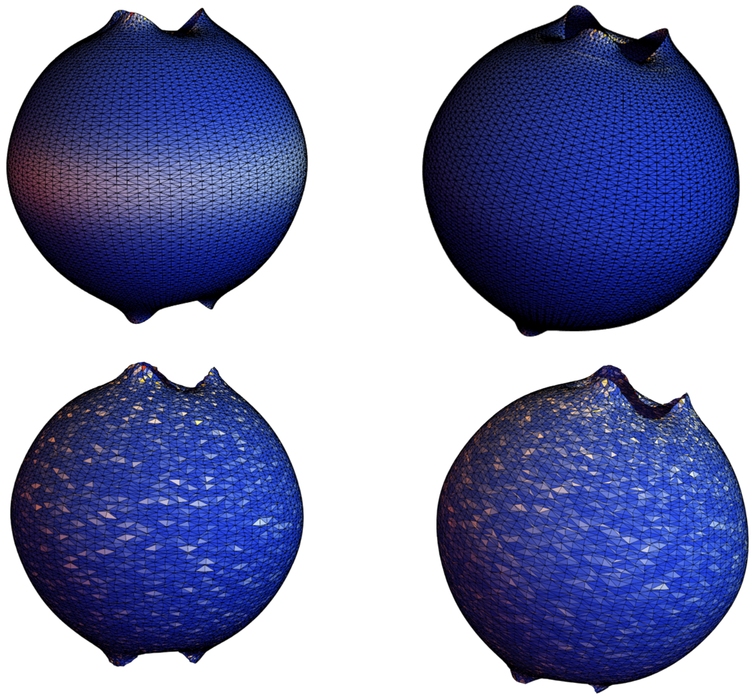

Figure 2: This example was constructed by growing the sphere conformally using the conformal factor $\Omega \propto \cos(3\phi)\exp\left[\frac{\theta-\pi/2}{\pi/10}\right]$. The top two spheres represent the results after optimization, while the bottom two spheres represent the results for a random initial registration. The left side shows the conformal factor, while the right side shows the shear deformation. Note that the shear is negligible compared to the dilation as expected.

registration will not involve any in plane displacements, thus minimizing distortion. Whether this property is desirable depends on the physical problem. We will test the behaviour of this algorithm using several constructed examples (Figs. 1, 2).

May be used later

A rate of deformation of a surface $\mathbf{X}(\mathbf{u}, t)$ can be decomposed into tangent and normal components as

$$\mathbf{V}(\mathbf{u}, t) \equiv \partial_t \mathbf{X}(\mathbf{u}, t) = V^k(\mathbf{u}, t)\, \mathbf{e}_k(\mathbf{u}, t) + V^n(\mathbf{u}, t)\, \hat{\mathbf{N}}(\mathbf{u}, t). \tag{14}$$

The corresponding change in the metric is given by

$$\partial_t g_{ij}(\mathbf{u}, t) = \nabla_i V_j(\mathbf{u}, t) + \nabla_j V_i(\mathbf{u}, t) - 2\, V^n(\mathbf{u}, t)\, b_{ij}(\mathbf{u}, t). \tag{15}$$

The normal displacement, or velocity $V^n(\mathbf{u}, t)$, will be referred to as gauge invariant because it does not depend on the registration. The parts that depend on the registration are the tangent displacements.

VI. ALGORITHM FOR FINITE DEFORMATIONS AND SHAPE CLASSIFICATIONS

The algorithm presented in the previous two sections suffers from some drawbacks. First, the distance function cannot be easily extended since for fast computation the gradient and hessian need to be given. Second as seen in the previous section correlations between curvature (or any other field defined on the surface) and growth can be destroyed in the registration algorithm. We can overcome this difficulty by adding to the cost function terms that prefer correlation between the growth fields and other given fields on the surface.

These problems maybe overcome if we use smooth representations of the surface, like moving least square (MLS) approximations. And use basis functions, like Fourier series, to write an arbitrary diffeomorphism $\mathbf{y}(\mathbf{u})$.

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[1] Anuj Srivastava and Eric Klassen, *Functional and Shape Data Analysis*, Springer, New York, (2016)