

Construction of differentiable transformations

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ABSTRACT

Construction of invertible transformations using differential equations is an interesting and challenging mathematical problem with important applications. We briefly review the existing method by means of harmonic maps in 2D and propose a method of constructing differentiable, invertible transformations between domains in two and three dimensions. Preliminary numerical results demonstrate the effectiveness of the method.

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1. Introduction

The existence and numerical construction of invertible transformations using differential equations constitute an interesting and challenging mathematical problem. A classic theorem [1] states that any harmonic map from a domain in R^2 to a convex domain in R^2 must be injective if it is one-to-one and onto between the boundaries. It is a natural question whether this is true in R^3 . It turns out that its extension to R^3 is false. In fact, Melas [2] constructed a harmonic map from a unit ball into another unit ball that is one-to-one and onto between the boundaries, but for which the Jacobian determinant is zero at the center. Later, this counterexample was modified in [3] such that it maps two distinct points to the same point.

As indicated in [4], the main obstacle to the harmonic map approach in three dimensions is demonstrated by Hans Lewy's counterexample of spherical harmonics of [5], whose nodal surface divides the sphere into exactly two components.

Since the Laplacian of a real-valued function w , Δw , can be expressed as $\text{div grad } w$, the Poisson equation $\Delta w = f$ is equivalent to the special div-curl system for $u = \text{grad } w$: $\text{div } u = f$ and $\text{curl } u = 0$. We adopted Moser's deformation method [6] from differential geometry and developed a div-curl-ODE (ordinary differential equation) system, which solves the direct problem (see Section 2). This system consists of a divergence equation, a curl equation, and an ordinary differential equation (ODE). The div and curl equations are solved to determine a suitable "velocity" vector field and the ODE determines a transformation from the velocity vector field. The main property of the transformation is that its Jacobian determinant has a prescribed (positive) value. This implies that the transformation is invertible if its restriction to the boundary is one-to-one and onto. In this work, we review the div-curl-ODE method for construction of invertible transformations from D_1 to D_2 with prescribed Jacobian determinant, where D_1 and D_2 are domains in R^d , $d = 2, 3$, and D_2 is not required to be convex. We will then focus on the "inverse" problem of reconstructing any given differentiable and invertible transformation using such a system, and the use of this div-curl-ODE system as the constraint for a large class of important optimization problems which requires an effective modeling of local motions (or displacements). We will describe the direct problem of

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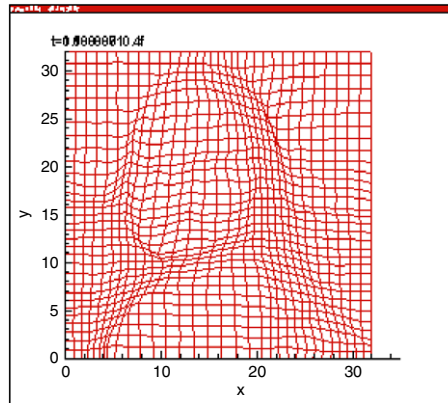


Fig. 1.1. Left: $\text{curl } u = g = 0$.

constructing a transformation in Section 2. Then we study the inverse problem in Section 3 and formulate a new approach to image registration in Section 4. Numerical examples are presented in Section 5. For simplicity of presentation, we take $D_1 = D_2 = D$, which is $[0, 1]^2$ in R^2 or $[0, 1]^3$ in R^3 .

2. Construction of a transformation with prescribed Jacobian determinant

Let $f > 0$ be any given function normalized to satisfy $\int f = |D|$. We construct an invertible transformation φ such that its Jacobian determinant at each $\mathbf{x} = (x, y, z)$ in D , $J(\varphi(\mathbf{x}))$, equals $f(\mathbf{x})$. This problem is solved both theoretically and computationally. The solution method is based on Jurgen Moser's work on volume elements of Riemannian manifolds [6]. The main technical advance made in [7] is that we use div-curl in place of the Poisson equation, which enables the treatment of moving domains. It turns out that the flexibility provided by the curl equation can be explored in the reconstruction of any given invertible transformation (see Example 1).

Solution method: For a given function $f(\mathbf{x}) > 0$ with $\int f = |D|$, we take $f(\mathbf{x}) - 1$ as the right hand side of the div equation (remark: the resulting divergence equation is the linearization of the equation $J(\varphi) = f$). Then we take any divergence free vector field g (i.e. $\text{div } g = 0$) as the right hand side of the curl equation. We solve for a vector field u from the div-curl equations:

$$\text{Div } \mathbf{u}(\mathbf{x}) = f(\mathbf{x}) - 1$$

$$\text{Curl } \mathbf{u}(\mathbf{x}) = g(\mathbf{x}) \quad \text{with } \mathbf{u} \bullet n = 0, n = \text{the outward normal on } \partial D.$$

Then, we form a velocity vector $\mathbf{v}(\mathbf{x}, t)$:

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}) / (t + (1 - t)f(\mathbf{x})) \quad \text{for a parameter } t \text{ in } [0, 1], \mathbf{x} \text{ in } D.$$

Now we solve a family of transformations $T(\mathbf{x}, t)$, t in $[0, 1]$, from the ordinary differential equation (ODE) for each fixed \mathbf{x} in D :

$$\partial T(\mathbf{x}, t) / \partial t = \mathbf{v}(T(\mathbf{x}, t), t) \quad \text{with } T(\mathbf{x}, 0) = \mathbf{x}.$$

Finally, we define φ by setting $\varphi(\mathbf{x}) = T(\mathbf{x}, 1)$.

It is shown in [8] that under reasonable smoothness assumptions, we do indeed have $J(\varphi(\mathbf{x})) = f(\mathbf{x})$. In particular, $J(\varphi(\mathbf{x})) > 0$, which in turn implies that T is invertible.

Notes: (1) This construction solves the nonlinear problem $J(\varphi(\mathbf{x})) = f(\mathbf{x})$ by solving linear partial differential equations, an algebraic relation for the "velocity" vector, and an ODE of Lagrange type in fluid mechanics. (2) $J(\varphi)$ is not influenced by g , which does change the transformation φ (see Example 1 below). (3) It is valid in both 2D and 3D domains, and the target domains need not be convex. (4) The method can be modified to treat domains with moving boundary [7].

Example 1 (Effect of the Curl). Transformations can be visualized on a grid. The two grids below are generated from the div-curl -ODE system described above with the same f that is proportional to the gradient of the intensity of a Mona Lisa image. The grid on the left is generated with $g = 0$, the right one with $g \neq 0$ in a region on the forehead of the portrait. Since the Jacobian determinants of each of the transformations are equal to the same function f , the cell size distributions of the two grids are the same. But the two transformations are different: the gridlines on the forehead of the right image are rotated due to the non-zero curl (Figs. 1.1 and 1.2).

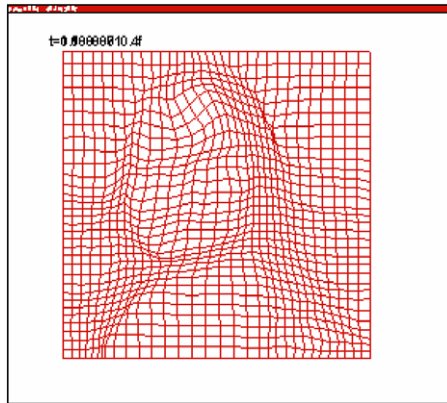


Fig. 1.2. Right: $\text{curl } u = g \neq 0$.

3. Reconstruction of the invertible transformation

3.1. A method based on the div-curl-ODE system

Let $S(\mathbf{x})$ be a given invertible transformation on D . The inverse problem is to express S as $T(\mathbf{x}, 1)$ with $T(\mathbf{x}, t)$ satisfying a div-curl-ODE system. This formulation is suitable for our optimal control formulation for the motion modeling problem described in Section 4.

We need to determine f and g from S . Determination of f is straightforward, since f would be equal to the Jacobian determinant of S . Thus, we compute $J(S)(\mathbf{x})$, and then set $f(\mathbf{x}) = J(S)(\mathbf{x})$. Direct determination of g is quite challenging. Instead, we determine $g(x)$ by minimizing $\int |T(\mathbf{x}, 1) - S(\mathbf{x})|^2$ over all possible g . More precisely, in order to determine g , we solve the following optimal control problem with $f(\mathbf{x})$ determined above:

Min $\int |T(\mathbf{x}, 1) - S(\mathbf{x})|^2$ over all g with $\text{div } g = 0$ in the following div-curl-ODE system:

$$\text{Div } \mathbf{u}(\mathbf{x}) = f(\mathbf{x}) - 1$$

$$\text{Curl } \mathbf{u}(\mathbf{x}) = g(\mathbf{x}) \quad \text{with } \mathbf{u} \bullet n = 0, \quad n = \text{the outward normal on } \partial D,$$

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}) / (t + (1 - t)f(\mathbf{x})) \quad \text{for } t \text{ in } [0, 1]$$

$$\partial T(\mathbf{x}, t) / \partial t = \mathbf{v}(T(\mathbf{x}, t), t) \quad \text{with } T(\mathbf{x}, 0) = \mathbf{x}.$$

The analysis and numerical method for addressing this problem have been studied in [9]. This reconstruction method may apply to image registration (see Section 4 below), which is the process of establishing a point-by-point correspondence between two images of a scene.

3.2. A method based on div-curl with preliminary numerical results

A simpler method is now formulated for reconstructing a given transformation on a simple domain such as a square or a cube. In this subsection, we reconstruct differentiable transformations using only the div-curl equations. The least squares finite element method is used to approximate the equations.

For a given transformation on a uniform initial grid we can calculate its divergence and curl at each point. Thus we can set up a div-curl system of equations for each point. Solving this system on the grid, we can reconstruct the given transformation. This idea can be used to reconstruct any differentiable and invertible transformation.

We will first take a look at the div-curl system. Let D be an open bounded domain in R^3 with a piecewise smooth boundary $\Gamma = \Gamma_1 \cup \Gamma_2$. Let (x, y, z) denote a point in D . Let $F = P \vec{i} + Q \vec{j} + R \vec{k}$ be a vector field in D . Let \vec{n} be the unit outward normal vector on the boundary. Then the 3D div curl system of equations is

$$\begin{cases} \text{div } F = \alpha & \text{in } D \\ \text{curl } F = \vec{\beta} & \text{in } D \\ \vec{n} \cdot F = 0 & \text{on } \Gamma_1 \\ \vec{n} \times F = 0 & \text{on } \Gamma_2 \end{cases} \quad (3.1)$$

where $\vec{\beta} = \beta_1 \vec{i} + \beta_2 \vec{j} + \beta_3 \vec{k}$.

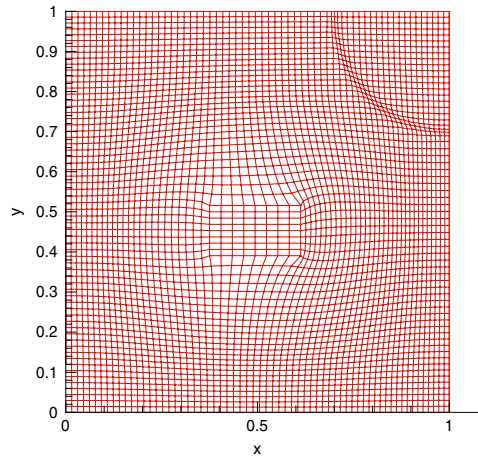


Fig. 2.1. The given transformation.

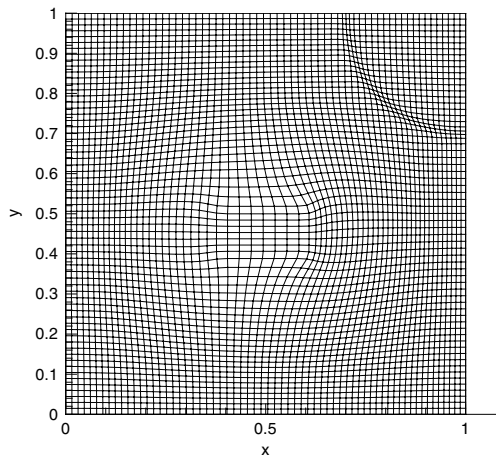


Fig. 2.2. The reconstructed transformation.

Our goal is to solve for P, Q, R , for a total of three unknowns. But we have four scalar equations in this system. So, it appears that this system is ‘overdetermined’. This system is shown (see [10]) to be equivalent to (3.2) which is obtained by introducing a dummy drill variable θ , where $\theta \equiv 0$ in D and $\theta = 0$ on Γ_1 :

$$\begin{cases} \operatorname{div} F = \alpha & \text{in } D \\ \nabla \theta + \operatorname{curl} F = \vec{\beta} & \text{in } D \\ \vec{n} \cdot F = 0 & \text{on } \Gamma_1 \\ \theta = 0 & \text{on } \Gamma_1 \\ \vec{n} \times F = 0 & \text{on } \Gamma_2 \end{cases} \quad (3.2)$$

(3.2) now has four unknowns and it has a unique solution.

Next, we present two numerical examples. Let the coordinates of the new position of node X_i be XN_i . We define $\text{Error} = \max |XN_i - X_i| = \sqrt{(xn_i - x_i)^2 + (yn_i - y_i)^2 + (zn_i - z_i)^2}$, $i = 1, \dots, k$. It is the maximal distance between each pair of corresponding nodes of the given and the reconstructed transformations. k is the maximum number of nodes. ‘Error’ is used to measure the accuracy of the reconstruction method.

The grid size of the following examples is 64×64 over the unit square $[0, 1] \times [0, 1]$ for 2D and $40 \times 40 \times 40$ over the unit cube $[0, 1] \times [0, 1] \times [0, 1]$ for 3D. That means the node spacing in the uniform grid is $\frac{1}{64} = 0.015625$ for 2D and $\frac{1}{40} = 0.025$ for 3D.

Example 2 (Reconstruction of a Transformation of Local Stretching and Rotation). A transformation from the uniform Cartesian grid (not shown) to a grid with a stretched rectangle and refined around an arc (Fig. 2.1) is reconstructed. Fig. 2.2 shows the reconstructed result.

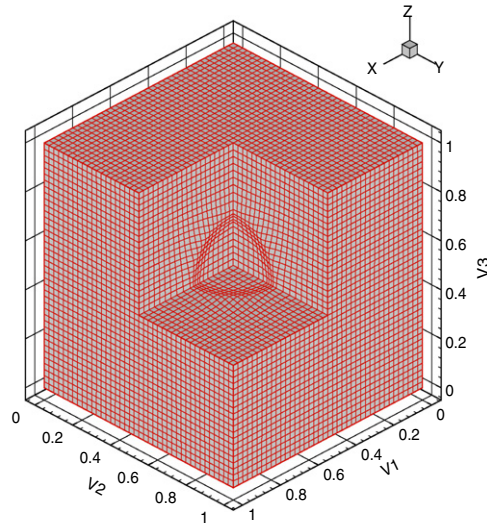


Fig. 3.1. The given transformation.

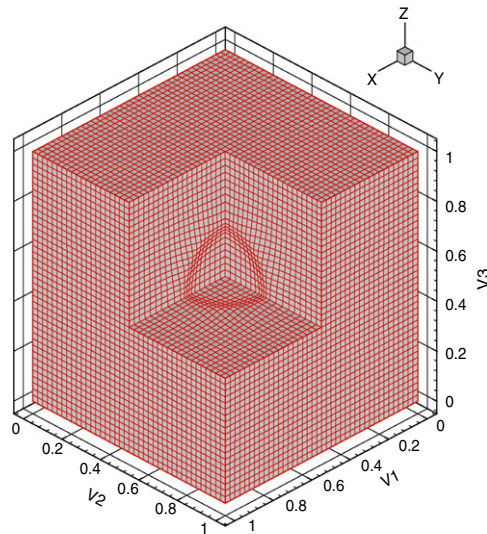


Fig. 3.2. The reconstructed transformation.

Example 3 (Three Dimensions). A transformation on the 3D Cartesian grid from a unit cube is shown in Fig. 3.1 using a grid adapted to a sphere. The reconstructed transformation is shown in Fig. 3.2. The maximum error is $\text{Error} = 5.225 \times 10^{-3}$, which is less than one quarter of the grid size $\frac{1}{40} = 0.025 = 25 \times 10^{-3}$.

4. Application to the image registration problem

On the basis of the solution method of Section 3, we formulate an optimal control approach to the image registration problem. For simplicity of presentation, we use the sum of squared differences (SSD) as the similarity measure: $\text{SSD} = \int (I_1(x, y, z) - I_2(\varphi(x, y, z)))^2$. Thus, we are seeking a transformation φ on the domain D such that a pixel (x, y, z) in I_1 is matched to the pixel $\varphi(x, y, z)$ in I_2 , and such that the sum of squared differences over all pixels is minimized subject to the constraint that φ is obtained from the div-curl-ODE system.

More precisely, to determine the displacement from a pixel at $\mathbf{x} = (x, y, z)$ in I_1 to a corresponding pixel in I_2 by $\varphi(\mathbf{x}) = T(\mathbf{x}, 1)$, we minimize $\text{SSD} = \int (I_1(\mathbf{x}) - I_2(T(\mathbf{x}, 1)))^2$ over all possible controls f and g with $f(\mathbf{x}) > 0$, $\int f = |D|$, and $\text{div } g = 0$, subject to the constraints

$$\begin{aligned} \text{Div } \mathbf{u}(\mathbf{x}) &= f(\mathbf{x}) - 1 \\ \text{Curl } \mathbf{u}(\mathbf{x}) &= g(\mathbf{x}) \quad \text{with } \mathbf{u} \bullet n = 0, n = \text{the outward normal on } \partial D, \\ \mathbf{v}(\mathbf{x}, t) &= \mathbf{u}(\mathbf{x}) / (t + (1 - t)f(\mathbf{x})) \quad \text{for } t \text{ in } [0, 1] \text{ and } \mathbf{x} \text{ in } D, \end{aligned}$$

where $\partial T(\mathbf{x}, t) / \partial t = \mathbf{v}(T(\mathbf{x}, t), t)$ for t in $[0, 1]$ and each fixed \mathbf{x} in D with initial condition $T(\mathbf{x}, 0) = \mathbf{x}$.

From the discussions in Sections 2 and 3, we conclude that the admissible space consists of all transformations that are differentiable and invertible. This approach has several advantages:

- (1) No regularization term is added to the SSD.
- (2) The PDE constraints are linear.
- (3) The method does not rely on feature extraction, but it can easily incorporate any available features.

Thus, the similarity measure can be accurately optimized by standard numerical optimization methods. This method has a solid mathematical foundation, since the minimizer exists (satisfying the constraints), and is unique.

The above optimal control method is simplified if we replace the div–curl–ODE system by the div–curl system described in Section 3.1. The simplified method is implemented through a least squares finite element method. Preliminary results are reported in [11].

5. Conclusions

Two methods of constructing invertible transformations are proposed. They are both based on the method of deformation for adaptive grid generation. The div–curl–ODE method can construct a transformation with prescribed Jacobian determinant. The main advantages of this approach are as follows:

- (1) The right hand side of the div equation has a clear geometric meaning: Suppose we want the Jacobian determinant to be a positive function $f(x, y, z)$, then we use $f - 1$ as the right hand side of the div equation.
- (2) Consequently, the natural constraint for f is simply $f > 0$ and $\int f = |D|$. These two properties make the div–curl–ODE system a natural constraint for optimization of similarity measures in the image registration problem described in Section 4.

In this work, the simpler method of reconstructing a given transformation based on div–curl equations is implemented through the least squares finite element method. Numerical examples in both two and three dimensions are presented. The examples show excellent accuracy of the method. The numerical method and examples based on the div–curl–ODE system will be reported in an upcoming paper.

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