

NON-RIGID REGISTRATION OF SHAPES VIA DIFFEOMORPHIC POINT MATCHING

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ABSTRACT

Diffeomorphic non-rigid registration of shapes is a very difficult problem. We use the point-set representation for shapes since statistical shape analysis in this space is relatively straightforward. Diffomorphic matching of point-sets requires an automated solution to the very difficult correspondence problem. We describe a joint clustering and diffeomorphism estimation strategy which allows us to simultaneously estimate the correspondence and fit a diffeomorphism between two unlabeled point-sets. Essentially, the cluster centers in each point-set are always in correspondence by virtue of having the same index. During clustering, the cluster center counterparts in each point-set are linked by a diffeomorphism and hence are forced to move in lock-step with one another. Experimental results are shown for 2D corpus callosum point-sets.

1. INTRODUCTION

The kernel of statistical shape analysis is the choice of distance measure for shape matching and registration. And, regardless of whether shapes are parameterized by points, lines, curves etc., at the heart of shape matching is the correspondence problem. When shapes are parameterized by point-sets, the statistical shape analysis problem is fairly straightforward. Means, covariances and even probability distributions on point-set manifolds can be defined and estimated [1]. However, the correspondence problem is particularly acute in the point-set representation since there is no natural *ordering* of the points that narrows down the set of allowed correspondences.

Recently [2, 3], there has been considerable interest in non-rigid point matching—the simultaneous estimation of point correspondences and non-rigid deformations between unlabeled point-sets. In *all* the prior work that we are aware of, the typical deformation model is a spline with thin-plate splines, Gaussian radial basis functions and B-splines being the most popular. The principal drawback of using a spline

for the spatial mapping or the deformation model is the inability of the spline to guarantee that there are no local folds or reflections in the mapping and that a valid inverse exists. In other words, a spline spatial mapping is not guaranteed to be a diffeomorphism.

In parallel to the above work on point correspondences is the recent work on *landmark diffeomorphisms* [4, 5]. Given two sets of landmarks or labeled point-sets, the aim here is to construct a diffeomorphism between them. Motivated by this work, we decided to combine the aforementioned work on point correspondences with this recent work on landmark diffeomorphisms to finally be able for the *very first time* to simultaneously estimate point correspondences and a diffeomorphism between unlabeled point-sets. In other words, the present work can be seen as automatically *estimating* landmarks and a smooth, differentiable, invertible spatial mapping between two unlabeled point-sets.

We follow recent work on joint clustering and matching [6] and imbibe the spirit of automated landmarking in our problem set up [7]. Rather than estimate point-to-point correspondences in the original point-sets, we establish correspondences between two sets of *cluster centers*. That is, correspondences exist only at the cluster center level and not at the level of the original point-sets. And, in an attempt to reduce the computational complexity of the resulting algorithm, we, in following the aforementioned joint clustering and matching strategy, decided to have a common index to the cluster centers in both point-sets. If the point-sets are independently clustered, then we have a new correspondence problem between two sets of cluster centers which may require having to estimate a permutation matrix. We wanted to avoid this complication. Instead, we simultaneously estimate the cluster centers in each point-set and estimate a diffeomorphism between the two sets of cluster centers. Since a cluster center in one point-set has a counterpart in the other, the diffeomorphism estimation is straightforward and directly follows the landmark diffeomorphism work mentioned above. Finally, since cluster centers in the two point-sets share a common index, during cluster center estimation, they are forced to move in lockstep by the diffeomorphism linking them. We use a standard, determin-

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istic annealing EM algorithm for cluster center estimation [6] with the main modification coming from the diffeomorphism force linking the two sets of cluster centers.

2. DIFFEOMORPHIC POINT MATCHING WITH UNKNOWN CORRESPONDENCE

We now describe the mathematical framework of diffeomorphic point matching. Given two point-sets $X = \{x_i | i = 1, \dots, N_1\}$ and $Y = \{y_j | j = 1, \dots, N_2\}$ in a region Ω of a 2-D plane, our goal is to find the best diffeomorphism $f : \Omega \rightarrow \Omega$ that maps the point-set X onto the point-set Y . The best diffeomorphism is that mapping which has the least deformation of the space Ω . Since correspondence is only defined at the cluster center level, the diffeomorphism maps cluster center counterparts in each set onto the other. Counterpart cluster centers have the same index.

We begin with an objective function which characterizes the diffeomorphic point matching problem. It consists of i) a clustering sub-objective for each point-set, ii) a coupling sub-objective which binds cluster center counterparts via the diffeomorphism and iii) a landmark diffeomorphism sub-objective. We describe each sub-objective below.

The clustering sub-objective uses a standard squared Euclidean distance between points and cluster centers with a cluster membership matrix (unknown until estimated) weighing each distance term. This objective function is

$$E_{\text{cluster}}(\mathbf{M}^x, \mathbf{r}) = \sum_{i=1}^{N_1} \sum_{k=1}^C M_{ik}^x \|x_i - r_k\|^2 \quad (1)$$

where $M_{ik}^x \in \{0, 1\}$ and $\sum_{k=1}^C M_{ik}^x = 1$. The matrix M^x is the membership of data point x_i in cluster k whose center is at the position r_k . A similar clustering subobjective holds for point-set Y . The clustering problem is strictly defined by this objective function and we don't discuss this problem in the context of mixture models. Consequently, we have no information theoretic restriction on the number of cluster centers C at present. Since the clustering will be constrained by the diffeomorphism, standard MDL like terms for the number of cluster centers C are inappropriate. We have empirically found that a larger number of cluster centers than is typical for *unconstrained* clustering gives the best results. so that we don't have a restriction regarding the number of cluster centers C . The number of cluster centers C can be any number greater than or equal to one. We use the well known deterministic annealing EM algorithm [6] to solve this clustering problem. In the annealing algorithm, we work with continuous memberships $0 < M_{ik} \leq 1$. We start with a high temperature and at each iteration, we reduce temperature and update the memberships and the positions of cluster centers. At the end, the position of cluster centers will converge to the limit positions and the memberships will converge to values close to $\{0, 1\}$ and together

will minimize the objective function. When the number of cluster centers is equal to the number of points, $C = N$, there is an obvious solution to minimize the objective function.

The coupling sub-objective which links the cluster counterparts is

$$E_{\text{coupling}}(\mathbf{r}, \mathbf{s}, f) = \sum_{k=1}^C (\|s_k - f(r_k)\|^2 + \|r_k - f^{-1}(s_k)\|^2) \quad (2)$$

where the function f and f^{-1} are the spatial mappings generated by the diffeomorphism. This coupling objective makes cluster center counterparts s_k and r_k influence each other via the diffeomorphism.

Finally, the landmark diffeomorphism sub-objective is

$$E_{\text{diff}}(\mathbf{q}, v) = \sum_{k=1}^C \int_0^1 \left\| \frac{dq_k(t)}{dt} - v(t, q_k(t)) \right\|^2 dt + \lambda \int_0^1 \int_{\Omega} \|Lv\|^2 dt dx \quad (3)$$

with the condition that $q_k(0) = s_k$ and $q_k(1) = r_k$. The end points of the landmark objective are the cluster centers. The main twist from the landmark matching perspective is that the end points themselves are unknown and need to be determined via clustering. In (3), $v(t, x)$ is an independent variable which is close to the tangent at $q_k(t)$, namely $\frac{dq_k}{dt}$ and is a smooth mapping. The first term ensures that v is close to the tangent and the second term ensures that v is smooth. For more details and a proof that minimizing (3) generates a diffeomorphism, please see[4]. The overall mapping f is a diffeomorphism that maps Ω to Ω . It is generated by a velocity field $v(t, x)$. $f(x) = \varphi(1, x)$ and φ is the solution to $\frac{d\varphi(t, x)}{dt} = v(t, \varphi(t, x))$, $t \in [0, 1]$ and $\varphi(0, x) = x$.

The overall objective function is

$$E(\mathbf{M}^x, \mathbf{M}^y, \mathbf{r}, \mathbf{s}, \mathbf{q}, v) = E_{\text{cluster}}(\mathbf{M}^x, \mathbf{r}) + E_{\text{cluster}}(\mathbf{M}^y, \mathbf{s}) + E_{\text{coupling}}(\mathbf{r}, \mathbf{s}, f) + E_{\text{diff}}(\mathbf{q}, v) \quad (4)$$

3. A JOINT CLUSTERING AND DIFFEOMORPHISM ALGORITHM

The joint clustering and diffeomorphism estimation algorithm has two components, i) clustering and ii) diffeomorphism estimation. As mentioned previously, the clustering of the two point-sets is handled by a deterministic annealing EM algorithm which iteratively estimates the cluster memberships \mathbf{M}^x and \mathbf{M}^y and the cluster centers \mathbf{r} and \mathbf{s} . The memberships update is the very standard E-step of the EM algorithm [6] and is performed as shown below.

$$M_{ik}^x = \frac{\exp(-\beta \|x_i - r_k\|^2)}{\sum_{l=1}^C \exp(-\beta \|x_i - r_l\|^2)}, \quad (5)$$

$$M_{jk}^y = \frac{\exp(-\beta\|y_j - s_k\|^2)}{\sum_{l=1}^C \exp(-\beta\|y_j - s_l\|^2)} \quad (6)$$

where $\beta = \frac{1}{T}$ is the inverse temperature. The cluster center update is the M-step of the EM algorithm. This step is not the typical M-step. We use a closed-form solution for the cluster centers which is an approximation. From the clustering standpoint, we assume that the change in the diffeomorphism at each iteration is *sufficiently small so that it can be neglected*. After making this approximation, we get

$$r_k = \frac{\sum_{i=1}^{N_1} M_{ik}^x x_k + f^{-1}(s_k)}{1 + \sum_{i=1}^{N_1} M_{ik}^x}, \quad (7)$$

$$s_k = \frac{\sum_{j=1}^{N_2} M_{jk}^y y_j + f(r_k)}{1 + \sum_{j=1}^{N_2} M_{jk}^y}, \forall k. \quad (8)$$

With the landmarks r_k and s_k held fixed, we use Camion and Younes' algorithm [4] to find the best $\mathbf{q}(t)$ and $v(t, x)$. Please refer to their work for more details. Essentially, we use a Green's function expansion for the smoothness term of the velocity field and run gradient-descent on $\mathbf{q}(t)$ and $v(t, x)$ until convergence. A thin-plate spline is used for the linear operator L . The overall algorithm is described below.

- **Initialization:** Initial temperature $T = 0.5(\max_i \|x_i - x_c\|^2 + \max_j \|y_j - y_c\|^2)$ where x_c and y_c are the centroids of X and Y respectively.
- **Begin A:** While $T > T_{\text{final}}$
 - **Step 1:** Clustering
 - Update memberships according to (5)(6).
 - Update cluster centers according to (7)(8).
 - **Step 2:** Diffeomorphism
 - Update (\mathbf{q}, v) by minimizing

$$E_{\text{diff}}(\mathbf{q}, v) = \sum_{k=1}^C \int_0^1 \left\| \frac{dq_k(t)}{dt} - v(t, q_k(t)) \right\|^2 dt + \lambda \int_0^1 \int_{\Omega} \|Lv\|^2 dt dx$$
 - **Step 3:** Annealing. $T \leftarrow \gamma T$ where $\gamma < 1$.
- **End**

4. EXPERIMENTS AND RESULTS

We used nine 2D corpus callosum slices. The feature points were extracted with the help of a neuroanatomical expert. We used 68 cluster centers in all experiments. Figure 1 shows the nine corpus callosum 2D images. The clustering of two sets of corpus callosum point-sets [point-set in (1,3) is matched to point-set (3,3) from point-set matrix in Figure 1] is shown in Figure 2. The circles represent the centers and the dots are the data points. The correspondences

(at the cluster level) are shown in Figure 3 with the diffeomorphic warping of space shown in Figure 4. A second example [(1,2) matched to (2,1)] of a diffeomorphic warping of space is shown in Figure 5. From the original nine corpus callosum point-sets, we warped the first eight point-sets onto the ninth set and Figure 6 displays the final overlay of all point-sets after diffeomorphic warping.

5. CONCLUSIONS

We have presented a joint clustering and diffeomorphism estimation algorithm in this paper. To our knowledge, this is the first effort aimed at diffeomorphic point matching. While other diffeomorphism methods exist for curves etc., this is not the case for unlabeled point-sets. In the present work, we finesse the notorious point correspondence problem via a simultaneous clustering and diffeomorphism estimation approach. Since cluster centers with the same index are always in correspondence, this considerably alleviates the correspondence problem. We were able to force the corresponding cluster centers to move in lockstep by explicitly coupling them in the objective function. The result is a constrained clustering algorithm where the diffeomorphism constrains the cluster center movement in one step and the cluster centers act as landmarks in the second diffeomorphism estimation step. We plan to further refine the coupling term in our joint clustering and diffeomorphism estimation approach in future work. Extension to atlas estimation is also straightforward.

6. REFERENCES

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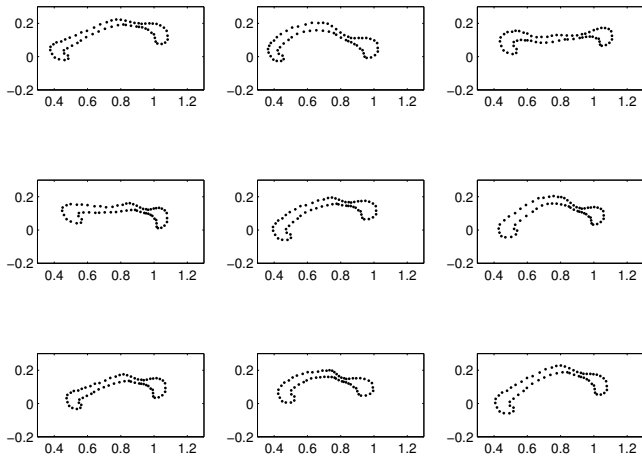


Fig. 1. Point sets of nine corpus callosum images.

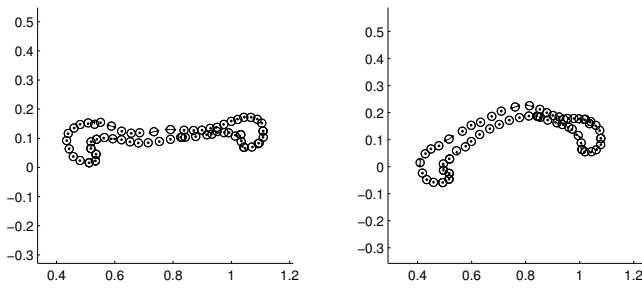


Fig. 2. Clustering of the two point sets.

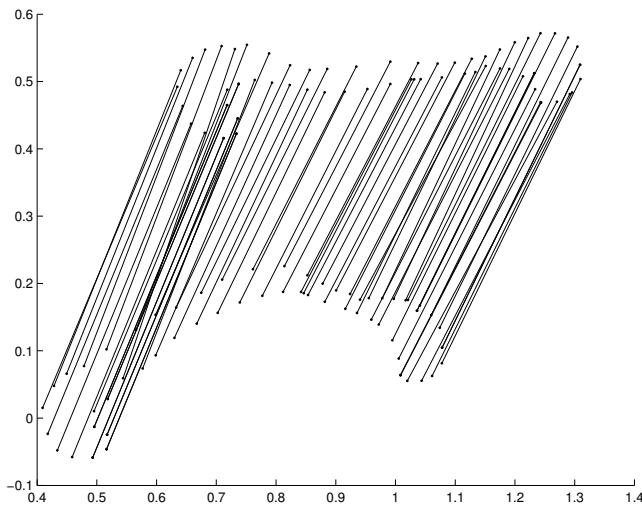


Fig. 3. Matching between the two point sets.

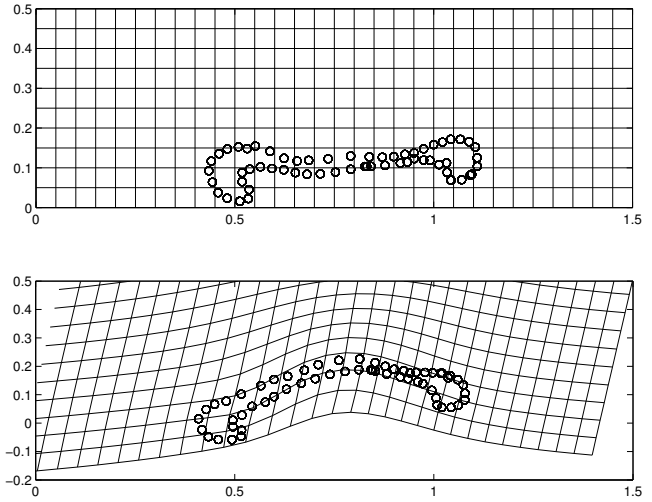


Fig. 4. Diffeomorphic mapping of the space.

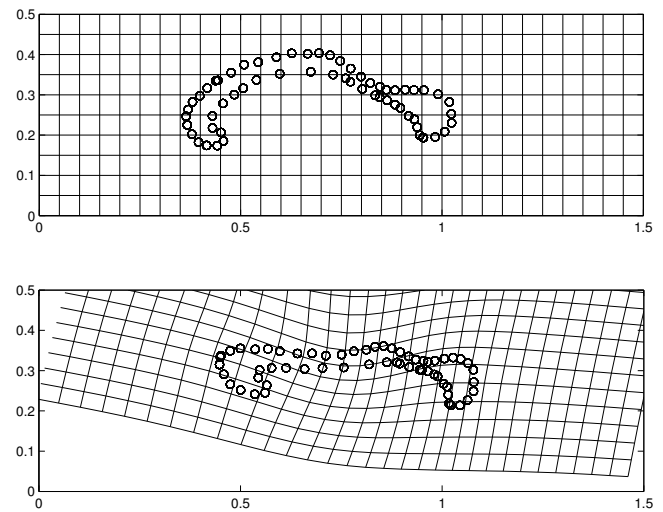


Fig. 5. Diffeomorphic mapping of the space.

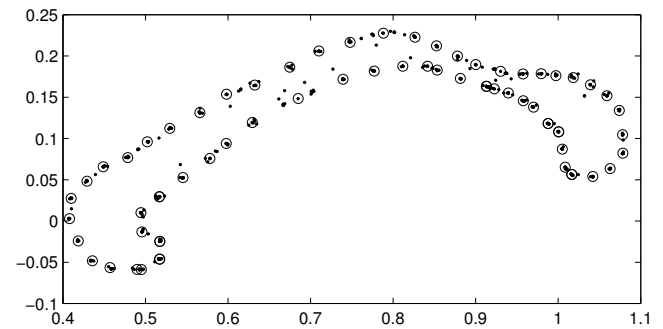


Fig. 6. Overlay of the after-images of eight point sets with the ninth set.