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To cite this version:
Claire Cury, Joan Alexis Glaunès, Marie Chupin, Olivier Colliot. Fast Template-based Shape Analysis using Diffeomorphic Iterative Centroid. MIUA 2014 - Medical Image Understanding and Analysis 2014, Jul 2014, Egham, United Kingdom. pp.39-44. hal-01050590

HAL Id: hal-01050590
https://inria.hal.science/hal-01050590
Submitted on 25 Jul 2014

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Fast Template-based Shape Analysis using Diffeomorphic Iterative Centroid

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Abstract

A common approach for the analysis of anatomical variability relies on the estimation of a representative template of the population, followed by the study of this population based on the parameters of the deformations going from the template to the population. The Large Deformation Diffeomorphic Metric Mapping framework is widely used for shape analysis of anatomical structures, but computing a template with such framework is computationally expensive. In this paper we propose a fast approach for template-based analysis of anatomical variability. The template is estimated using a recently proposed iterative approach which quickly provides a centroid of the population. Statistical analysis is then performed using Kernel-PCA on the initial momenta that define the deformations between the centroid and each subject of the population. This approach is applied to the analysis of hippocampal shape on 80 patients with Alzheimer’s Disease and 138 controls from the ADNI database.

1 Introduction

Computational Anatomy aims at developing tools for the quantitative analysis of variability of anatomical structures, and its variation in healthy and pathological cases \([8]\). A common approach in Computational Anatomy is template-based analysis, where the idea is to compare anatomical objects variations relatively to a common template. These variations are analysed using the ambient space deformations that match each individual structure to
the template. The Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework [1] has been widely used for the study of the geometric variation of human anatomy. This framework generates metrics between deformable shapes and provides smooth and non ambiguous matchings between objects.

Estimating a template from the population in the LDDMM framework, to be used for further template-based statistical analysis, is a computationally expensive task. Several methods have been proposed. Vaillant et al. proposed in 2004 [12] a method based on geodesic shooting which iteratively updates a shape by shooting towards the mean directions. The method proposed by Glauñès and Joshi [7] starts from the whole population and estimates a template by co-registering all subjects using a backward scheme. A different approach was proposed by Durrleman et al. [4, 5]. The method initializes the template with a standard shape, and uses a forward scheme: deformations are defined from the template to the subjects. The method presented by Ma et al. [9] uses an hyper template which is an extra fixed shape, and optimizes at the same time deformations from the hyper template to the template and deformations from the template to subjects of the population. All these methods are expensive in terms of computation time, due to the iterations needed for the convergence of the method.

In this paper, we propose a fast approach for template-based shape analysis in the LDDMM framework. The template is estimated using an iterative approach which quickly provides a centroid of the population [3]. This method iteratively computes a centroid of the population in the LDDMM framework, which requires only \( N - 1 \) matching steps, with \( N \) the number of subjects, while template estimation methods typically require \( N \) such steps per iteration. Using this centroid computation as initialization drastically reduces the computation time for template computation. We use this iterative centroid as a template to study the anatomical variability by analysing the deformations from the centroid to the subjects of the population using Kernel-PCA [10]. This approach was applied to 218 hippocampi (80 patients with Alzheimer’s Disease, 138 controls) from the Alzheimer’s Disease Neuroimaging Initiative (ADNI) database 1.

2 Methods

2.1 LDDMM framework

We briefly present the LDDMM framework to introduce notations, for more details see [1]. Deformation maps \( \varphi : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \) are generated via integration of time-dependent vector fields \( v(x,t), x \in \mathbb{R}^3, t \in [0,1] \), such that each \( v(\cdot,t) \) belongs to a Reproducing Kernel Hilbert Space \( V \) with kernel \( K_V \). The transport equation

\[
\begin{cases}
\frac{d\phi_v}{dt}(x,t) = v(\phi_v(x,t),t) & \forall t \in [0,1] \\
\phi_v(x,0) = x & \forall x \in \mathbb{R}^3
\end{cases}
\]

has a unique solution, and one sets \( \varphi_v = \phi_v(\cdot,1) \) the diffeomorphism induced by \( v(x,t) \).

In a discrete setting, optimal vector fields \( v(x,t) \) are expressed as combinations of spline fields: \( v(x,t) = \sum_{p=1}^{n} K_V(x,x_p(t)) \alpha_p(t) \), where \( x_p(t) = \phi_v(x_p,t) \) are the trajectories of control points \( x_p \) (the vertices of the mesh to be deformed), and \( \alpha_p(t) \in \mathbb{R}^3 \) are time-dependent vectors called momentum vectors. Optimal trajectories between shapes can be shown to

1(adni.loni.usc.edu). The Principal Investigator of this initiative is Michael W. Weiner, MD, VA Medical Center and University of California - San Francisco.
satisfy geodesic equations for a metric on the set of control points [12]. As a result the full deformation between a template shape and its surface target $S_i$ is encoded by the vector of initial momentum vectors $\alpha^i(0) = (\alpha_p^i(0))_{1 \leq p \leq n_i}$ located on the vertices of the template mesh.

### 2.2 Iterative Centroid method

We proposed in 2013 [3] an Iterative Centroid method which use the LDDMM framework and the framework of currents [11]. The authors propose three different schemes for centroid computation, but here we only use the first one, which is the faster one. The Iterated Centroid method consists in applying the following procedure: given a collection of N shapes $S_i$, we first set $C_1 = S_1$ (initial centroid) and successively update the centroid by matching it to the next shape and moving it along the geodesic flow. (Algorithm 1).

**Data:** $N$ surfaces $S_i$

**Result:** 1 surface $C_N$ representing the centroid of the population

$C_1 = S_1$;

for $i$ from 1 to $N - 1$ do

- $C_i$ is matched to $S_{i+1}$ which results in a deformation map $\phi_{i+1}(x, t)$;
- Set $C_{i+1} = \phi_{i+1}(C_i, \frac{1}{i+1})$ which means we transport $C_i$ along the geodesic and stop at time $t = \frac{1}{i+1}$;

end

**Algorithm 1:** Iterative Centroid algorithm

This algorithm can be defined in a pure Riemannian setting, for the averaging of a set of points $p_k$ (instead of shapes $S_i$) on a Riemannian manifold $M$. If points $p_k$ belong to a vector space and the metric is flat, the algorithm converges towards the mean $\frac{1}{N} \sum_k p_k$, but in general it depends on the ordering of the points. Back to our shape space framework, we showed in a previous study [3] that indeed the ordering changes the result, but the different results are very close to each other. Emery and Mokobodzki [6] proposed to define the centroid not as a unique point but as the set $\mathcal{C}_N$ of points $p \in M$ satisfying $f(p) \leq \frac{1}{N} \sum_{k=1}^{N} f(p_k)$, for any convex function $f$ on $M$ (a convex function $f$ on $M$ being defined by the property that its restriction to all geodesics is convex). This set $\mathcal{C}_N$ takes into account all centroids obtained by bringing together points $p_k$ by all possible means, i.e. recursively by pairs, or by iteratively adding a new point, as we are doing with Algorithm 1. To further reduce the computational load, we used a GPU implementation for the kernel convolutions involved in the matchings.

### 2.3 Statistical Analysis

For the statistical analysis of shapes, we compute a centroid of the population, and we use it as a template. Then we deform the centroid toward each shape of the population to obtain the deformations from the centroid to the population. The deformations are determined by the vector of initial momentum vectors $\alpha^i(0)$; we can analyse these deformations with a Kernel-PCA [10] as in [12]. The Kernel-PCA is the non-linear version of the Principal Component Analysis (PCA) which can be used for learning shape variability from a training set, or for reducing dimensionality of the shape space. In fact the difference between the two versions is in the computation of the covariance matrix, which writes
\[ \text{Cov}(i, j) = \frac{1}{N-1} \left( \alpha^i(0) - \bar{\alpha}(0) \right) K_V(x)(\alpha^j(0) - \bar{\alpha}(0)), \]
with \( \bar{\alpha}(0) \) the mean of initial momentum vectors and \( K_V(x) \) the matrix of the \( K_V(x^i, x^j) \). Then we can run a standard PCA on the covariance matrix \( \text{Cov} \).

### 3 Experiments and results

#### Dataset

The method was applied to the analysis of hippocampal shape of 80 patients with Alzheimer’s Disease (AD) and 138 controls (CN) (\( N = 218 \)) from the Alzheimer’s Disease Neuroimaging Initiative (ADNI) database. Left hippocampi were segmented with the SACHA software (Chupin et al. [2]) from 3D T1 weighted MRI. Then the meshes were computed using the BrainVisa \(^2\) software. They are composed of 800 vertices on average.

#### Results

We computed a centroid for each of the two populations (AD and CN) using Algorithm 1. The two centroids are denoted \( \text{IC}(AD) \) and \( \text{IC}(CN) \). Computation times were 2.4 hours for \( \text{IC}(AD) \) and 3.6 hours for \( \text{IC}(CN) \). To assess whether the centroids are close to the center of the respective population, we computed the ratio

\[ R = \frac{\| \frac{1}{N} \sum_{i=1}^{N} v_0(S_i) \|_V}{\| \frac{1}{N} \sum_{i=1}^{N} \| v_0(S_i) \|_V} \]

between the mean of the norms of initial vector fields from the centroid to the population and the norm of the mean of initial vector fields. Both ratios are 0.25, which means that both centroids are correctly centred even though they are not exactly at the Fréchet mean (which would correspond to \( R = 0 \)). To visualise differences between \( \text{IC}(CN) \) and \( \text{IC}(AD) \), we computed distances between vertices (figure 1) of \( \text{IC}(CN) \) and the deformation of \( \text{IC}(CN) \) on \( \text{IC}(AD) \).

![Figure 1: Distances between IC(CN) and IC(AD). On the left, the hippocampus is viewed from below.](http://www.brainvisa.info)

We then analysed the variability of the AD and the CN populations using Kernel-PCA. Figure 2 shows, for each group, the principal mode of variation. This figure is obtained by geodesic shooting from each centroid in the first principal direction with a magnitude of \( \pm 2\sigma \). One can note that, while the templates of the two groups are different, the variabilities of both groups share similarities. Nevertheless, there seems to be less variability in the medial part of the body for the CN group.

In order to visualize the localization of \( \text{IC}(CN) \) and \( \text{IC}(AD) \) and their modes within the whole population, we computed a centroid of the whole population and performed the corresponding K-PCA. We then projected \( \text{IC}(CN) \) and \( \text{IC}(AD) \) on the two first principal

\(^2\)http://www.brainvisa.info
Figure 2: First mode of deformation of the AD group (top) and of the CN group (bottom). For each row, the centroid is in the center (in blue), on the right its deformation at $+2\sigma$, and at $-2\sigma$ on the left. The colormap indicates the displacement of each vertex between the corresponding centroid and its deformation.

components. We can observe (figure 3) that $IC(CN)$ is on the left of the global centroid, and $IC(AD)$ is on the right, and the 3 principal modes of variation have different directions.

Figure 3: First principal modes of the whole population (in green). In blue, the projections of $IC(CN)$ and projections of its deformations at $\pm 2\sigma_{CN}$ in the direction of its first mode of variation. In red, for the AD group. Intermediate points are show the trajectory of the first modes.

4 Conclusion

In this paper, we proposed a new approach for fast template-based shape analysis in the LDDMM framework. The template is estimated using a diffeomorphic iterative centroid method. The Iterative Centroid is roughly centred within the population of shapes. Analysis of variability is then based on a Kernel-PCA of the initial momenta that define the deformations of the template to each individual. We applied this approach to the analysis of hippocampal shape in AD patients and control subjects. Projection of the templates of the CN group and the AD group onto the main modes of variability of the whole population show that they are located on the main axis of variability. The template estimation takes only a
couple of hours for both populations (with about 100 subjects each). The low computational load of the proposed approach makes it applicable to very large datasets.

Acknowledgments

The research leading to these results has received funding from ANR (project HM-TC, grant number ANR-09-EMER-006, and project KaraMetria, grant number ANR-09-BLAN-0332) and from the program Investissements d’avenir ANR-10-IAIHU-06.

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