A New Shape Diffusion Descriptor for Brain Classification

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Abstract. In this paper, we exploit spectral shape analysis techniques to detect brain morphological abnormalities. We propose a new shape descriptor able to encode morphometric properties of a brain image or region using diffusion geometry techniques based on the local *Heat Kernel*. Using this approach, it is possible to design a versatile signature, employed in this case to classify between normal subjects and patients affected by schizophrenia. Several diffusion strategies are assessed to verify the robustness of the proposed descriptor under different deformation variations. A dataset consisting of MRI scans from 30 patients and 30 control subjects is utilized to test the proposed approach, which achieves promising classification accuracies, up to 83.33%. This constitutes a drastic improvement in comparison with other shape description techniques.

1 Introduction

Brain morphology techniques using Magnetic Resonance Imaging (MRI) are playing an increasingly important role in understanding pathological structural alterations of the brain [1,2]. A typical approach is to investigate the presence of morphological differences of selected brain structures between neuropsychiatric patients and healthy controls [2]. To this aim, methods for shape analysis can be exploited in order to extract the geometric information which provides the best statistical performance in separating the two populations (i.e., healthy and non-healthy people)[3]. Classic approaches evaluate volumetric variations [2] to explain atrophy or dilation due to such kind of illnesses. Nevertheless, more advanced shape analysis techniques have been proposed aiming at exploiting new aspects of the shape such as spectral [4,5] or local geometric properties [6]. A typical methodology consists of encoding such geometric properties into a *descriptor* which compactly represents the shape. In this fashion, the comparison between shapes can be carried out by measuring the descriptors' similarities in

G. Fichtinger, A. Martel, and T. Peters (Eds.): MICCAI 2011, Part II, LNCS 6892, pp. 426–433, 2011.

the descriptor space. Thus, the effectiveness of shape descriptors can be evaluated in terms of discriminativeness and robustness against shape variations due to noise or deformations.

In this paper, we propose a new shape descriptor based on advanced *diffusion* geometry techniques. Local geometric properties are encoded by the so-called *Heat Kernel* [7] which exploits heat diffusion characteristics at different scales. The general idea consists of capturing information about the neighborhood of a point on the shape by recording the dissipation of heat over time from that point onto the rest of the shape. In this way, *local* shape characteristics are highlighted through the behavior of heat diffusion over short time periods, and, conversely, *global* shape properties are observed while considering longer periods [7,8]. So doing, simply varying a single parameter (the time), it is possible to characterize the properties of a shape at different scales. Therefore, local heat kernel values observed at each point are accumulated into a histogram for a fixed number of scales leading to the so-called *Global Heat Kernel Signature* (GHKS).
The method is inspired by [7] which proposed the *Heat Kernel signature* (HKS) for a single vertex of a mesh. Here, we extend the HKS for the whole shape for both surface mesh (i.e., external surface) and volumetric representation. The proposed descriptor has several nice properties which are shared with very few other work. GHSK allows for shape comparisons using minimal shape preprocessing, in particular, no registration, mapping, or remeshing is necessary. GHKS is robust to noise since it implicitly employs surface smoothing by neglecting higher frequencies of the shape. Finally, GHKS is able to encode isometric invariance properties of the shape [7] which are crucial to deal with shape deformations.

The proposed descriptor has been tested in the context of the analysis of the schizophrenia illness. A Region-of-Interest (ROI)-based approach [1] is employed by studying the left-thalamus, which is known to be impaired by such disease [2]. Experiments, carried out on a dataset of 30 patients and 30 controls, lead to promising classification results in distinguishing between the two populations also in comparison with other methods.

2 Related Work

Several work has been proposed for detecting alterations of the brain structure by using advanced shape analysis techniques [4,6]. A common approach consists of capturing *global* shape information from the (shape-)spectral domain [5,4]. In [5], geometric properties are encoded by computing spherical harmonic descriptors (SPHARM) on brain surfaces. Although results are interesting, the method is not invariant to surface deformations and therefore it requires shapes registration and data resampling. This pre-processing is avoided in [4], where the so called Shape-DNA signature has been introduced by taking the eigenvalues of the Laplace-Beltrami operator as region descriptor for both the external surface and the volume. Although *global* methods can be satisfying for some classification tasks, they do not provide information about the localization of the morphological anomalies. To this aim, *local* methods have been proposed.

In [6] the so called *feature*-based morphometry (FBM) approach is introduced. Taking inspiration from feature-based techniques proposed in computer vision, FBM identifies a subset of features corresponding to anatomical brain structures that can be used as disease biomarkers. Other approaches are able to combine both *global* and *local* information. More specifically, a recent and important class of methods has been introduced for generic object analysis which employs heat diffusion procedures on 3D shapes [7,8,9,10]. In this class of techniques, global information is provided by the spectral parameters of the Laplace-Beltrami operator employed on 3D data, and local information is defined by the heat diffusion at small scales. In [7], Sun et al. have proposed the so called *Heat Kernel Signature*(HKS): the main idea was to describe the diffusion from a point to itself at several time instants. The HKS provides a natural and efficiently computable multi-scale way to capture information about neighborhoods of a given point. A similar approach has been proposed in [8] by introducing the so called *Auto Diffusion Function* (ADF). The idea and formulation is the same as in [7], but the procedure has been applied for object segmentation and skeleton extraction. In order to obtain a global signature from local measures two main strategies has been proposed [10,9]. In [9] the well known *Bag-of-features* approach is employed starting from the HKS value at each point of the shape. Coversely, in [10] the global shape is captured by computing the distribution of diffusion distances among the points of the shape. In [9], a study on isometry-invariance property of the geometric diffusion process is proposed in order to highlight the differences between *volume*-isometry and *boundary*-isometry. In the former case, the diffusion is computed at voxel level, whereas in the latter the diffusion is computed only on the external surface.
Our approach extends the use of heat kernel on MRI data for classification purposes on medical domain. The method proposed improves [5] since our descriptor is isometry invariant. Moreover, differently than [4], our approach implements a multi-scale analysis to increase the discriminativeness properties of the descriptor. Finally, the main idea of the heat kernel signature[7] to describe the diffusion from a point to itself at different scales has been revised to work on global shape.

3 The Heat Diffusion Process

Given a shape M as a compact Riemannian manifold, the heat diffusion on shape[1] is defined by the *heat* equation:

$$(\Delta_M + \frac{\partial}{\partial t})u(t,x) = 0; \tag{1}$$

where u is the distribution of heat on the surface, Δ_M is the *Laplace-Beltrami* operator which, for compact spaces, has discrete eigendecomposition of the form $\Delta_M = \lambda_i \phi_i$. In this fashion the *heat kernel* has the following eigendecomposition:

$$k_t(x,y) = \sum_{i=0}^{\infty} e^{-\lambda_i t} \phi_i(x)\phi_i(y), \tag{2}$$

[1] In this section, we borrow the notation from [7,9].

where λ_i and ϕ_i are the i^{th} eigenvalue and the i^{th} eigenfunction of the Laplace-Beltrami operator, respectively. The heat kernel $k_t(x, y)$ is the solution of the heat equation with point heat source at x at time $t = 0$, i.e., the heat value at point y after time t. The heat kernel is *isometric invariant*, it is *informative*, *multi-scale*, and *stable* [7]. In order to estimate the Laplace-Beltrami and the heat kernel in discrete domains several strategies can be employed [9]. In the following we describe the cases of surface meshes and volumetric representations.

Heat kernel on surface meshes. In the case of surface mesh only the boundary of the shape is considered. In order to work on a discrete space, we estimate the Laplace-Beltrami operator by employing linear Finite Elements Methods (FEM) [4]. More in detail, given a triangular mesh composed by $v_1, \cdots, v_m$ vertices, with *linear* finite elements the *generalized eigendecomposition* problem [4] becomes:

$$A_{cot}\Phi = -\Lambda B\Phi, \tag{3}$$

where Λ is the diagonal matrix of the Laplace Beltrami eigenvalues λ_i, and Φ is the matrix of corresponding eigenfunctions ϕ_i. The matrices A_{cot} and B are defined as:

$$A_{cot}(i,j) = \begin{cases} \frac{cot\alpha_{i,j} + cot\beta_{i,j}}{2} & if \quad (i,j) \in E, \\ -\sum_{k \in N(i)} A_{cot}(i,k) & if \quad i = j, \\ 0 & otherwise. \end{cases} \tag{4}$$

$$B(i,j) = \begin{cases} \frac{|t_1| + |t_2|}{12} & if \quad (i,j) \in E, \\ \frac{-\sum_{k \in N(i)} |t_k|}{6} & if \quad i = j, \\ 0 & otherwise. \end{cases} \tag{5}$$

where E is the set of edges of the triangular mesh, $\alpha_{i,j}$ and $\beta_{i,j}$ are the two angles opposite to the edge between vertices v_i and v_j in the two triangles sharing the edge (i, j), $|t_i|$ is the area of the triangle t_i, and t_1, t_2 are the triangles that shares the edge (i, j). Indeed, the *heat kernel* can be approximated on a discrete mesh by computing Equation 2 and retaining the k smallest eigenvalues and the corresponding eigenfunctions.

Heat kernel on volumetric representations. In the case of volumetric representations, the interior part of the shape is also considered. The volume is sampled by a regular Cartesian grid composed of voxels, which allows the use of standard Laplacian in R^3 as the Laplace-Beltrami operator. We use finite differences to evaluate the second derivative in each direction of the volume. The heat kernel on volumes is invariant to volume isometries, in which shortest paths between points inside the shape do not change. Note that in real applications exact volume isometries are limited to the set of rigid transformations [9]. However, also non-rigid deformations can faithfully be modelled as approximated volume isometries in practice. Moreover, differently from spectral surface representation, volumetric approach is able to capture volume atrophy. It is worth noting that, as observed in [7,9], for small t the heat kernel $k_t(x,x)$ of a point x with itself is directly related to the *scalar* curvature $s(x)$ [9]. More formally:

$$k_t(x,x) = (4\pi t)^{-3/2}(1 + \frac{1}{6}s(x)). \quad (6)$$

Note that in the case of surface meshes $s(x)$ can be interpreted as the Gaussian curvature [7]. In practice, Equation 6 states that heat tends to diffuse slower at points with positive curvature, and viceversa. This gives an intuitive explanation about the geometric properties of $k_t(x,x)$ an leads the idea of using it to build a shape descriptor [7].

4 The Proposed Method

The proposed approach is composed of three main phases: i) data gathering, ii) estimation of descriptors, and iii) classification.

Data Gathering. Quantitative data collection and processing in MRI based research implies facing several methodological issues to minimize biases and distortions. The standard approach to deal with these issues is following well established guidelines dictated by international organizations, such as the World Health Organization (WHO), or codified by respected institutions, such as leading universities. In this work we employ a ROI-based approach [1]: only a well defined brain subpart has been considered. Specifically, we focus our analysis on the left-Thalamus whose abnormal activity is already investigated in schizophrenia. Regions have been manually traced by experts, according to well defined medical protocols.

Global Heat Kernel Signature. Once data are collected, a strategy to encode the most informative properties of the shape M can be devised. To this end, a global shape descriptor is proposed, which is inspired by the so-called *Heat Kernel Signature*(HKS) defined as:

$$HKS(x) = [k_{t_0}(x,x), \cdots, k_{t_n}(x,x)]. \quad (7)$$

where x is a point of the shape (i.e., a vertex of a mesh or a voxel) and $(t_0, t_1, \cdots, t_n)$ are n time values. To extend this approach to the whole shape, we introduce the following global shape descriptor:

$$GHKS(M) = [hist(K_{t_0}(M)), \cdots, hist(K_{t_n}(M))], \quad (8)$$

where $K_{t_i}(M) = \{k_{t_i}(x,x), \forall x \in M\}$, and $hist(\cdot)$ is the histogram operator. Note that our approach combines the advantages of [10,9] since it encodes the distribution of local heat kernel values and it works at multiscales. Figure 1 shows a schema of the proposed descriptor. Each point of the shape is colored according to $k_{t_i}(x,x)$. Such values are collected into a histogram for each scale t_i. Finally, histograms are concatenated leading to the global signature.

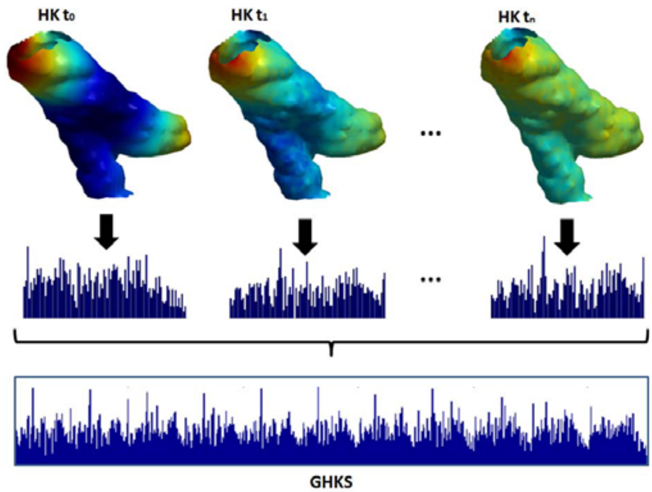

Fig. 1. GHKS: Each point of the shape is colored according to $k_{t_i}(x, x)$. Such values are collected into a histogram for each scale t_i. Finally, histograms are concatenated leading to the global signature.

Support Vector Machine Classification. These descriptors are simply evaluated using a Support Vector Machine (SVM), which is one of the most powerful classifier for object recognition [11]. SVM constructs a maximal margin hyperplane in a high dimensional feature space, by mapping the original features through a kernel function. Here, the input of the SVM are the set of GHKS descriptors extracted for each subject. A learning by example approach is introduced by adopting leave-one-out cross-validation procedure[2].

5 Results

The proposed shape classification method is employed for Schizophrenia detection in Thalamic region. A dataset composed of 30 male patients and 30 male controls has been evaluated. MRI scans were acquired using a 1.5 T Siemens Magnetom Symphony Maestro Class, Syngo MR 2002B. After manual extraction of the ROIs both mesh surfaces and volumetric representations have been recovered. The Laplace-Beltrami operator has been computed as described in Section 3, for both representations, and the *heat kernel* has been computed. In this work, we have used $k = 200$ eigenvalues, and we have scaled the temporal domain logarithmically in $n = 10$ time values, as suggested in [7]. Finally, the GHKS is computed by fixing 100 bins for each histogram. Therefore, for each

[2] A single sample is used as validation data, and the remaining samples as training data. The procedure is repeated such that every sample in the dataset is used once as validation data.

Table 1. Classification rates. The accuracy is computed by Leave-One-Out cross-validation. Three kernels are evaluated and two methods are compared. Both surface and volumetric representations are considered.

Method	Linear-SVM	Polynomial-SVM	RBF-SVM
Surface GHKS	65.00%	66.67%	71.67%
Volumetric GHKS	81.67%	80.00%	**83.33%**
Surface ShapeDNA	50.00%	66.67%	70.00%
Volumetric ShapeDNA	50.00%	71.67%	73.33%

subject the final dimension of the GHKS is $10 \cdot 100 = 1000$. The classification procedure is employed as described in Section 4. Several kernels have been evaluated, namely *linear*, *polynomial* (degree=3), and *radial basis function* (RBF). We compare our descriptor with the so called ShapeDNA descriptor, recently proposed by Reuter et al. [4]. As mentioned above, the ShapeDNA has similar properties of our GHKS descriptor since it encodes the *intrinsic* properties of the shape. Conversely, ShapeDNA does not deal with multiple scales and takes into account of only global information. Table 1 shows the classification performance of the considered approaches. The proposed GHKS descriptor clearly outperforms the ShapeDNA descriptor[3]. Specifically, a drastic improvement is observed when the volumetric approach is employed. In fact, volumetric GHKS reaches the best accuracy (i.e., 83.33%), and it is stable by varying the type of kernel employed. It is worth noting that also in the case of ShapeDNA, better performances are observed with the volumetric procedure. Therefore, from this study we can argue that volumetric approach is more suitable to deal with natural shape variations that raise on brain subparts of different subjects. The computational cost of the proposed GHKS descriptor is not high and effective: the Laplace-Beltrami transform can be employed in around 10 seconds for a mesh of about 3000 vertices. The same eigendecomposition on our volumetric data of $21 \times 37 \times 29$ voxels takes around 25 seconds. Then, the computation of final GHKS takes around a second for both the approaches[4].

6 Conclusions

In this paper, a new shape morphometry approach is introduced to improve the classification between normal subjects and patients affected by schizophrenia. Our GHKS descriptor combines local shape properties into a global signature by exploiting geometric diffusion procedure on MRI data. The approach proposed outperforms previous work, namely ShapeDNA, it is easy to be implemented and efficient. Both volumetric and surface approaches have been evaluated by showing that in our study neuroanatomical variations between different subjects are well modelled by volume isometries. From our experiments, we can highlight

[3] The same number of eigenvalues have been employed.

[4] We used a laptop at $1.66Ghz$. The code is written in Matlab with some parts in C.

the discriminativeness property of the thalamus by confirming the importance of this region to figure out mental disorders, especially in schizophrenia. Future work will address the localization of the disease on both surface and volume by further exploiting the local properties of the heat kernel on MRI data.

Acknowledgements. We acknowledge financial support from the FET programme within the EU-FP7, under the SIMBAD project (contract 213250).

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