Unsupervised clustering using Diffusion Maps for Local Shape Modelling

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Abstract. Understanding the biological variability of anatomical objects is essential for statistical shape analysis and to distinguish between healthy and pathological structures. Statistical Shape Modelling (SSM) can be used to analyse the shapes of sub-structures aiming to describe their variation across individual objects and between groups of them [1]. However, when the shapes exhibit self-similarity or are intrinsically fractal, such as often encountered in biomedical problems, global shape models result in highly non-linear shape spaces and it can be difficult to determine a compact set of modes of variation. In this work, we present a method for *local* shape modelling and analysis that uses Diffusion Maps [2] for non-linear, spectral clustering to build a set of linear shape spaces for such analysis. The method uses a curvature scale-space (CSS) description of shape to partition them into sets of self-similar parts and these are then linearly mixed to more compactly model the global shape.

Key words: Shape, Statistical Shape Modelling, Local Shape Models, Curvature Scale Space, Diffusion Maps, brain contours.

1 Introduction

Study of variability in natural objects has been a topic of research for many years. Different approaches have been used in this type of analysis, but since shape is one of the most important features of human perception it is natural to asses the variation in terms of it. In medicine, fundamental features of the brain structure or function (in health and disease) are revealed by digital imaging, but due to the complexity of the human brain, quantitative analysis is a challenging area of research [3]. Computational Anatomy is a discipline where the objective is to create algorithmic tools to help in the analysis of biological and anatomical structures, in particular, brain substructure. Identification of structural brain changes is associated with different neuro-degenerative diseases, so identifying such variation can bring valuable information in the diagnosis and treatment of many pathologies [4].

Statistical Shape Modelling (SSM) can be used to analyse the shapes of sub-structures aiming to describe their variation across individual objects and

between groups of them [1]. *Active Shape Models* deal well with problems such as the size of the training set and the homology (point-to-point correspondences), but its important to point out that these models are successful in modelling large scale variations, but they struggle with the finer shape details. Shen *et al.* [5], presents a deformable model for segmentation and definition of point correspondences in brain images using an adaptive-focus deformable statistical model based on affine-invariant attribute vectors, minimisation of an energy function and PCA. Worthy of mention are the many techniques created to model the surface of the brain like [6] where a spherical topology mapping and topology correction are used to map accurately the cortex. Shape modelling has shown that shape variation can be successfully modelled as in [7], in which an approach for shape representation that utilises medial representations derived from a spherical harmonics boundary description to study Hippocampus schizophrenia described. Xue *et al.* [8] proposed an automatic segmentation algorithm for neonatal brain MRI using a knowledge based approach to identify and reduce the MLPV in an EM-MRF segmentation scheme.

When the shapes exhibit self-similarity or are intrinsically fractal, such as often encountered in biomedical problems, global shape models results in highly non-linear shape spaces and it can be difficult to determine a compact set of modes of variation. Depending on the application, one approach is to combine rigid shape models together with parametric non-linear deformation, but this can result in far too many degrees of freedom being used. Others have reported on the use of hierarchical analysis of such shapes. In this work, we present a method for *local* shape modelling and analysis that uses Diffusion Maps [2] for non-linear, spectral clustering to build a set of linear shape spaces for such analysis. The method uses a curvature scale-space (CSS) description of shape to partition shapes into sets of self-similar parts [9] and these are then linearly mixed to more compactly model the global shape. We present results on a set of leaves and brain contours to asses the veracity of the method.

2 Method

Our proposed local shape modelling method consists of creating a pose independent shape space where the local contour variability can be measured. The model is based on a Point Distribution Model [1] where each shape obtained from an image (figure 1-(a)) is represented by a set of labelled points (figure 1-(b)):

$$c = \{x_1, y_1, \ldots, x_k, y_k\} \tag{1}$$

Using the consistency of curvature extrema points of the Curvature Scale Space (figure 1-(c)) we proceed to derive a set of local partitions from each contour (figure 1-(d)) . The later will be explained in detail in the next section. Once that a set of meaningful partitions is ready to be analysed we need to compare the shapes, but in order to do this they need to be aligned with respect to a set of axes. Hence an affine alignment is performed over the set to eliminate pose variation (figure 1-(e)). As we select a reference shape, we need to align each

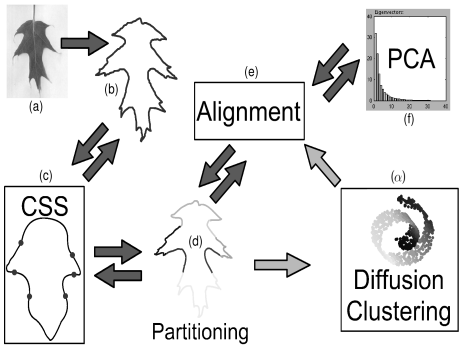

Fig. 1. Process for our local shape model: (a) The source image is processed so the contour (b) can be drawn out of it. Then the CSS process is applied in order to obtain the partitions of the contour (d). From here there are two flows, first we can proceed with the alignment (e) and finish with the PCA analysis (f) or we can proceed to (α) find a low-dimensional embedding of the sub-manifold using Diffusion Maps and k-means clustering to identify a set of local shape models

shape of the set with this one. Rigid body transformation parameters can be used to transform the points from any shape to the reference frame.

Here, we introduce the use of spectral clustering to build a set of linear shape spaces for such analysis (figure 1-(α)). We use the method described in [10] for extracting the intrinsic parameters of multiple shape classes in an unsupervised manner, where the method is based on learning the global structure of the shape manifolds [2].

2.1 Curvature Scale Space Zero-Crossings

A Curvature Scale Space is a technique for object representation, invariant under *pose* variations and based on the scale space representation. To build the CSS representation the curve needs to be considered as a parametric vector equation $\Gamma(t) = (x(t), y(t))$, then a series of *evolved versions* of $\Gamma(t)$ are produced by increasing the scale parameter, σ, from 0 to ∞. Every new evolved version is defined as $\Gamma_\sigma = (X(t,\sigma), Y(t,\sigma))$, where

$$X(t,\sigma) = x(t) \circledast g(t,\sigma) \ , \ Y(t,\sigma) = y(t) \circledast g(t,\sigma). \tag{2}$$

Here, $\circledast$ denotes the convolution operator and $g(t,\sigma)$ is a Gaussian of width σ. Since the CSS representation contains curvature zero-crossings or extrema points from the evolved version of the input curve, these are calculated directly from any Γ_σ by:

$$k(t) = \frac{\dot{X}(t,\sigma)\ddot{Y}(t,\sigma) - \dot{Y}(t,\sigma)\ddot{X}(t,\sigma)}{(\dot{X}(t,\sigma)^2 + \dot{Y}(t,\sigma)^2)^{3/2}} \tag{3}$$

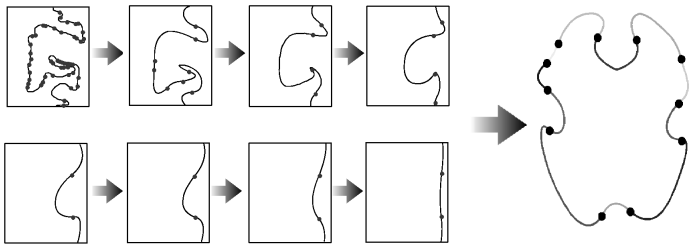

Fig. 2. CSS evolution of a white-matter brain contour. At some appropriate level of smoothing, a set of meaningful partitions can be identified. Pairs of zero-crossings (red points) are used to search and rank local parts on the original shape.

The final step is the construction of the CSS image, but only the generation of evolved versions of the curve and the locations of the curvature zero-crossings are relevant for this work, for further details see [11]. The generation of evolved versions of the curve, produces a set of zero-crossings of the second derivative where there is a change on the curvature of the contour. These points provide a basic but efficient way to create meaningful partitions contours that exhibit self-similar variation (Figure 2).

2.2 Shape representation

In the context of shape analysis is desirable to use a shape representation invariant to translation, rotation, and scale transformations. For this purpose Fourier descriptors (FD) where chosen to represent the shapes since they are effective for many problems of pattern classification and computer vision.

Let us regard any shape as a contour (closed curve) represented as a set of boundary points as in equation 1, then the *Centroidal distance* function is defined as the distance from the boundary points from the centroid of the shape: $r(i) = \sqrt{(x_i - \overline{x})^2 + (y_i - \overline{y})^2}$ where $\overline{x}$ and $\overline{y}$ denotes the coordinates of the centroid of the object. Then, the distance vector $r = \{r(1), r(2), \ldots, r(N)\}$ is transformed into the frequency domain using FFT. Now the feature vector $\mathbf{f}$ is derived as follows:

$$\mathbf{f} = \left(\frac{|F_1|}{|F_0|}, \frac{|F_2|}{|F_0|}, \cdots, \frac{|F_{N/2}|}{|F_0|} \right) \tag{4}$$

here $|F_i|$ denotes the *ith* Fourier coefficient and $|F_0|$ the *DC* component. In the last equation, due to the the fact that the centroidal distance function is real valued, only half of the FDs is needed to index the shape, as well, taking the magnitudes of the coefficients yields rotation invariance and scale invariance is obtained by dividing them by the DC component.

2.3 Shape manifolds and Diffusion Maps

Like most manifold learning methods, the first step of diffusion maps is to define the feature vectors, hence $\Omega = \{\mathbf{f}_1, \mathbf{f}_2, \ldots, \mathbf{f}_n\}$ (where n denotes the total of shapes) can be regarded as the set of feature vectors that corresponds to our data set of various shapes. Then as Ω regards these feature vectors as the nodes of the adjacency graph G such that $G = (\Omega, W)$, where W, the similarity matrix between $\mathbf{f}_i$ and $\mathbf{f}_j$ can be computed using the Gaussian kernel of width ε:

$$w(\mathbf{f}_i, \mathbf{f}_j) = e^{\frac{-||\mathbf{f}_i - \mathbf{f}_j||^2}{2\varepsilon}} \tag{5}$$

The graph G with weights W represents our knowledge of the local geometry of the set. Next, a Markov random walk is defined on this graph, and the degree of node $d(\mathbf{f}_i)$ of node $\mathbf{f}_i$ is expressed:

$$d(\mathbf{f}_i) = \sum_{z \in \Omega} w(\mathbf{f}_i, z) \tag{6}$$

Now, if P is defined as an $n \times n$ matrix whose entries are given by:

$$p_{ij} = \frac{w(\mathbf{f}_i, \mathbf{f}_j)}{d(\mathbf{f}_i)} \tag{7}$$

then $p(x, y)$ can be viewed as the transition kernel of a Markov chain on V.

As P contains geometric information about the data set, the transitions that it defines directly reflect the local geometry defined by the immediate neighbours of each node in the graph of the data. In other words, $p(i, j)$ represents the probability of transition from node i to node j in one time step [2]. Running the Markov chain forward is equivalent to computing powers of the operator P. For this computation, in theory, the eigenvalues and eigenvectors of P can be used, but instead, these objects can be directly employed in order to characterise the geometry of the data set. Hence, it is possible to define the family of diffusion maps $\{\Psi_t\}_{t \in \mathbb{N}}$ given by:

$$\Psi_t(x) \triangleq \begin{pmatrix} \lambda_1^t \psi_1(x) \\ \lambda_2^t \psi_2(x) \\ \vdots \\ \lambda_{s(\delta,t)}^t \psi_{s(\delta,t)} \end{pmatrix}. \tag{8}$$

Each component of $\psi_t(x)$ is termed *diffusion coordinate*. The mapping $\Psi_t : V \longrightarrow \mathbb{R}^{s(\delta,t)}$ embeds the data set into an Euclidean space of $s(\delta, t)$ dimensions.

3 Experimental Results

Our first experiments use closed contours. The data set was the same data set as in [10], six different shape classes from the Kimia database of object silhouettes.

The classes are: carriage (20 shapes), dog (49 shapes), rat (20 shapes), fish(32 shapes), hand (16 shapes) and horse (20 shapes) for a total of 157 samples (Figure 3-(b)). The next data set used for experimental evaluation had partitions from whole contours using the CSS zero-crossings 3 obtained from a set of leaf images. First, we used a set of 50 shapes of the leaf class Quercus Kelloggii, that generate approximately 600 leaf partitions, each partition was represented by 128 points. Corresponding results are presented in figure 3-(a). The brain contour data set for the following results was from McGill University's BrainWeb data of 20 anatomical models of normal brains ([12]). In this case, our data set consisted in 501 partitions coming from 60 white matter contours, and figure 3-(b) exhibit the results for this.

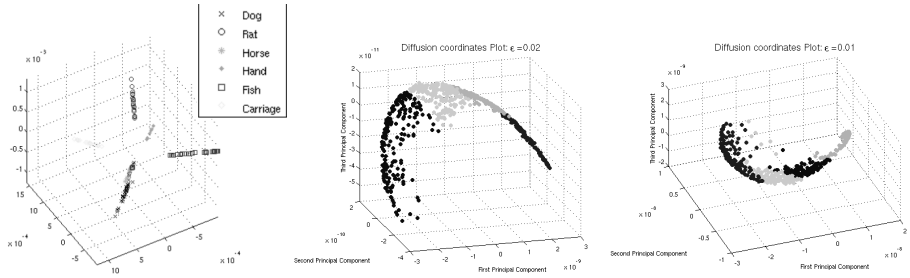

Fig. 3. Diffusion maps coordinates plots, results for contour shapes: (a) Kimia data set of six different classes of shapes: carriage, dog, rat, fish, hand and horse (b) 662 partitions from 50 leaf contours of the class Quercus Kelloggii and (c) 501 partitions from 60 white matter contours.

4 Evaluation and Discussion

The main contribution of this work is the creation of a method that obtains a set of meaningful shapes, meaning with that this that is possible to find local parts that are similar and localised according to a non-supervised the novel spectral clustering technique of Diffusion Maps. Furthermore, another objective of this idea was of generating ordered sets of partitions from contours is to establish a way of determining meaningful local sets of shapes. The spectral clustering is effective in discovering the non-linear manifold in the non-linear shape spaces. The combination of CSS and diffusion maps are a way to map from self-similar contours to a piece-wise shape description. We used spectral-clustering to build a set of 4 local (linear) shape models and then measure the reconstruction error for each model against a single (global) SSM. Figure 4 shows the cluster variation for the local versus global models and demonstrates the better compactness of the 4 classes over the global model.

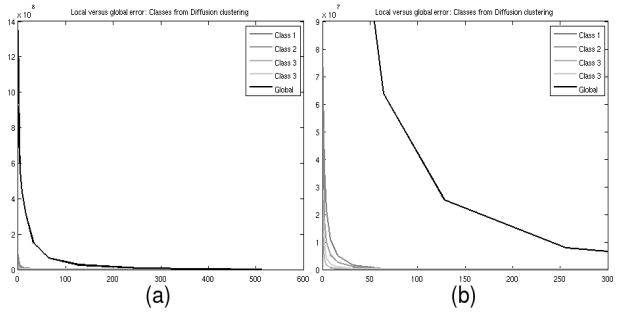

Fig. 4. Reconstruction log-error plot for the different clusters and for the global shape model in black.

The method has a number of applications in shape modelling of natural shapes, such as in biology and medical imaging. Elsewhere [9], we have described the latter shape model and with it, a simple windowing and blending technique which allows the modelled parts to be reconstructed back into the original global shape useful for visual feedback 5.

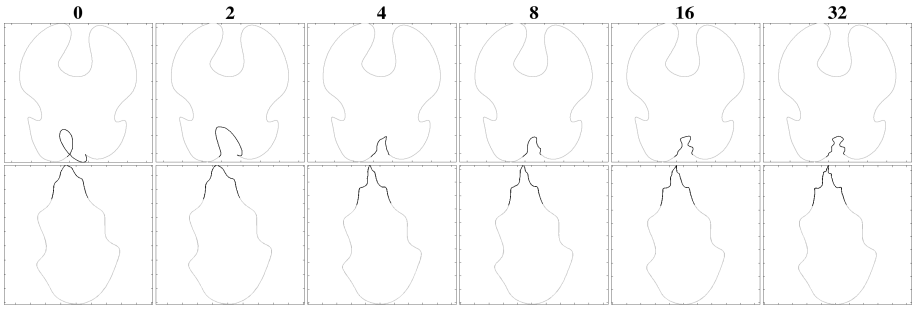

Fig. 5. Reconstruction of the chosen set of shapes, by added a sequence of principal modes of variation: 0, 2, 4, 8, 16, 32. First row corresponds to a white matter contour and second to a leaf from the class Quercus Kelloggii. The modelled partitions are blended back into a smooth scale of the CSS, Γ^{σ} defocussing the general, irrelevant shape variations for the purposes of visualisation.

The results presented here are illustrative and further validation is necessary. The method needs to be extended to surfaces to be properly validated with clinical data but it is not clear now how the local partitioning and the clustering could be easily extended to surface patches. We believe that that this model could have useful application in brain morphometrics and computational anatomy. To be more precise, the provided method could be adapted for clinical diagnosis

software for assessing changes in local shape variation of anatomical structures, such as, white/gray matter. Finally, the spectral clustering might be adapted for the problem of image database retrieval where the objective can be to discover images which contain objects similar to query objects, in this case brain sections.

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