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# UNSUPERVISED NONLINEAR CLUSTERING FOR SHAPE CORRESPONDENCES ANALYSIS

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## ABSTRACT

This paper proposes a method for shape correspondence analysis based on nonlinear unsupervised clustering.

100-150 palabras

## 1. INTRODUCTION

Correspondence problem in medical image analysis is a challenge research topic due to the importance of establish meaningful relations between any pair of brain structures (static registration problem) [14], or analyze temporal changes of a given neurodegenerative disease among time (dynamic analysis of brain structures) [7]. However, similarity measures that can capture common information between objects are difficult to obtain [5]. The main reason of this problem, relies on the fact that brain structures are nonrigid objects that exhibit morphological changes between subjects (brain volumetry over a population) and shape deformations over time in a neurodegenerative disease (i.e. Alzheimer and Parkinson) [6].

Analyzing brain structures properties, such as shape volumetry or cortical thickness, is an important task in Alzheimer's disease, due to the importance to monitoring these structures (i.e. hippocampus, thalamus, and ventricles), analyze anatomic connectivity, and finding disease patterns in the brain cortex [17, 8]. Nevertheless, the high variability of the brain patterns such as size, curved-ness and curvature, makes it necessary to compute the correspondences between objects in a group-wise manner [15].

Moreover, most of the correspondence methods for medical image problems are focused on computing different similarity metrics based on texture descriptors such as bag of words features [2], largest common point-sets [1] and geodesic contours [13]. However, most of these approaches only works on objects of the same size, which gives a poor accuracy in non-rigid matching processes, since a full relation of the matched features in all of their points is computed (point-to-point correspondence) [4].

In order to modeling the structure of a given object, methods for unsupervised object matching have been developed in the

last years. The aim of these methods is to establish meaningful correspondences in scenarios where shapes are described by non-rigid objects or the similarity measure between objects can not be computed [19]. Variational Bayesian matching [11] and Bayesian canonical correlation analysis [12] are some examples of these methods in which a given probabilistic framework is performed to model features between objects and establish the shape correspondences. Nonetheless, these methods only handles full correspondence frameworks (i.e. point-to-point matching) and linear analysis over the shape descriptors (i.e. appearance descriptors), which makes unsuitable to modeling shared information between non-rigid objects (i.e. tissue properties in MRI data) [18]. That is why this problem is still an open research topic in computer vision [6].

In this paper, we present a method for shape correspondences analysis based on nonlinear unsupervised clustering of group-wise 3D shape descriptors. The unsupervised clustering process is carried out by a kernelized probabilistic latent variable models, in which scale-invariant heat kernel signatures are used as 3D shape descriptors [3]. Our contribution relies on the kernelized version of the work proposed by Iwata [9], in which we extend the many-to-many object matching using Hilbert space embeddings of the brain structure shape descriptors [16]. The motivation of this method is based on the ability of modeling nonlinear objects in multiple domains, with different dimensionalities (i.e. brain structures in Alzheimer disease). We use an infinite Gaussian mixture model (iGMM) to assigning a latent vector for each descriptor with the aim to cluster objects (set of shape descriptors) in different brain structures, and to finding groupwise correspondences between clusters without using any similarity measure. The paper proceeds as follows. Section 2 presents the scheme for establishing the shape correspondences using nonlinear unsupervised clustering. Section 3 shows the experimental results, in which we report several experiments related to the probabilistic analysis of brain structures. The paper concludes in section 4 with some conclusions of the proposed method and future works.

## 2. MATERIALS AND METHODS

### 2.1. Database

In this work we used two MRI databases. First, a MRI database from the Technological University of Pereira (DB-UTP). This database contains MRI data from four patients with Parkinson’s disease, and it was labeled by the neurosurgery team from the Institute of Parkinson and Epilepsy of the Eje Cafetero, located in Pereira-Colombia. The database contains  $T1$ ,  $T2$  and  $CT$  sequences with  $1\text{ mm} \times 1\text{ mm} \times 1\text{ mm}$  voxel size and slices of  $512 \times 512$  pixels. Second, we use the SPL-PNL<sup>1</sup> Brain Atlas developed by the Surgical Planning Laboratory of Harvard Medical School, in collaboration with the Harvard Neuroscience Laboratory at Brockton VA Medical Center. The atlas was derived from a volumetric T1-weighted MR-scan of a healthy volunteer, using semi-automated image segmentation, and three-dimensional reconstruction techniques. The current version consists of: 1) the original volumetric whole brain MRI of a healthy volunteer; 2) a set of detailed label maps and 3) more than 160 three-dimensional models of the labeled anatomical brain structures.

### 2.2. Probabilistic Non-Linear Latent Variable Model for Groupwise Correspondence

In order to establish meaningful correspondences over a set of non-rigid 3D brain structures, our model is set as follows. First, we want to handling nonlinearities in the observed data (3D shape descriptors), the model sets that we are given shape descriptors for  $D$  domains  $\mathcal{X} = \{\mathbf{X}_d\}_{d=1}^D$  mapped to a Hilbert space  $\mathcal{H}$ , where  $\mathbf{X}_d = \{\mathbf{x}_{dn}\}_{n=1}^{N_d}$  is a set of objects in the  $d$ th domain, and  $\mathbf{x}_{dn} \in \mathbb{R}^{M_d}$  is the feature vector of the  $n$ th object in the  $d$ th domain. By introducing a function  $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$  called the *kernel*, that performs a given mapping over the objects,  $\phi : \mathcal{X} \rightarrow \mathcal{H}$  such that  $\forall x, x' \in \mathcal{X}, k(x, x') := \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$ , we can cluster groups of correspondences by using a non-linear function that represents the shape descriptors in the Hilbert space [16].

Secondly, we are unaware of any correspondences between shape descriptors in different brain structures. The number of descriptors  $N_d$  and the dimensionality  $L_d$  for each brain structure mapped in  $\mathcal{H}$  can be different from those of other structures. Therefore, our task is to match clusters of descriptors (groupwise correspondences) across multiple brain structures in an unsupervised manner using kernel methods [9, 16].

As in infinite Gaussian mixture models, our method assumes that we can find an infinite number of correspondences between objects in (clusters), and each cluster  $j$  has a latent vector  $\zeta_j \in \mathbb{R}^P$  in a latent space of dimension  $P$  in  $\mathcal{H}$ . De-

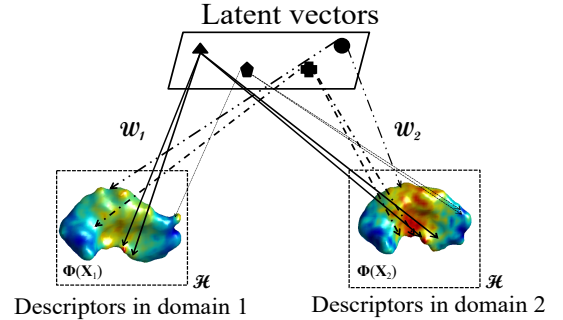
scriptors that have the same cluster assignments  $s_{dn}$ , are related by the same latent vector, which establishes the shape correspondence between brain structures.

Each object in  $\phi(\mathbf{x}_{dn}) \in \mathcal{H}$  in the  $d$ th domain is generated depending on the domain-specific projection matrix  $\mathcal{W}_d = [\varphi(\mathbf{w}_1^d), \varphi(\mathbf{w}_2^d), \dots, \varphi(\mathbf{w}_P^d)]$ ,  $\mathcal{W}_d \in \mathbb{R}^{L_d \times P}$  and latent vector  $\zeta_{s_{dn}}$  that is selected from a set of latent vectors  $\mathbf{Z} = \{\zeta_j\}_{j=1}^{\infty}$ . Here,  $s_{dn} = \{1, \dots, \infty\}$  is the latent cluster assignment of object  $\phi(\mathbf{x}_{dn})$ .

The proposed model is based on an infinite mixture model, where the probability of descriptor mapped in a Hilbert space  $\phi(\mathbf{x}_{dn})$  is given by

$$p(\phi(\mathbf{x}_{dn}) | \mathbf{Z}, \mathcal{W}, \theta) = \sum_{j=1}^{\infty} \theta_j \mathcal{N}(\phi(\mathbf{x}_{dn}) | \mathcal{W}_d \zeta_j, \alpha^{-1} \mathbf{I}), \quad (1)$$

where  $\mathcal{W} = \{\mathcal{W}_d\}_{d=1}^D$  is a set of projections matrices,  $\theta = (\theta_j)_{j=1}^{\infty}$  are the mixture weights,  $\theta_j$  represents the probability that the  $j$ th cluster is chosen and  $\alpha$  is a precision parameter. By employing projection matrices in Hilbert space for each brain structure (domain-specific), we can handling multiples structures with nonlinear properties (nonrigid shapes in medical imaging) and dimensionalities (i.e. size of the brain structures). Figure 1 shows the scheme of the proposed model, in which the relationship between shape descriptors in Hilbert space, and latent vectors is described.



**Fig. 1.** Scheme for the unsupervised nonlinear clustering method for groupwise correspondence analysis. The figure shows an example of establishing clusters of correspondences in Hilbert space for two brain structures (left putamen).

As in [10], we use a stick-breaking process to set the mixture weights for a Dirichlet process with concentration parameter  $\gamma$ , and then draw the cluster proportions.

The joint probability of the data  $\mathcal{X}$ , and the cluster assignments  $\mathbf{S} = \left\{ \{s_{dn}\}_{n=1}^{N_d} \right\}_{d=1}^D$  are given by

$$p(\Phi, \mathbf{S} | \mathcal{W}, a, b, r, \gamma) = p(\mathbf{S} | \gamma) p(\Phi | \mathbf{S}, \mathcal{W}, a, b, r). \quad (2)$$

<sup>1</sup>This database is available on <http://www.spl.harvard.edu/publications/item/view/1265>

where  $a, b$  and  $r$  are the hyperparameters.

By marginalizing out the mixture weights  $\theta$ ,  $p(\mathbf{S}|\gamma)$  becomes in

$$p(\mathbf{S}|\gamma) = \frac{\gamma^J \prod_{j=1}^J (N_{\cdot j} - 1)!}{\gamma(\gamma + 1) \dots (\gamma + N - 1)}, \quad (3)$$

where  $N = \sum_{d=1}^D N_d$  is the total number of shape descriptors,  $N_{\cdot j}$  represents the number of descriptors assigned to the cluster  $j$ , and  $J$  is the number of clusters that satisfies  $N_{\cdot j} > 0$ .

For our non-linear model, we give the derivation of the likelihood in (1), in which latent vectors  $\mathbf{Z}$  and precision parameter  $\alpha$  are analytically integrated out. To this end, we use two mappings functions  $\phi(\mathbf{x}_{dn})$  and  $\varphi(\mathbf{w}_j^d)$ , in order to represent our observations and projection matrices in the Hilbert space.

$$p(\Phi|\mathbf{S}, \mathbf{W}, a, b, r) = (2\pi)^{-\frac{\sum_d L_d N_d}{2}} r^{\frac{PQ}{2}} \frac{b^a}{b'^a} \times \frac{\Gamma(a')}{\Gamma(a)} \prod_{j=1}^Q |\Lambda_j|^{1/2}, \quad (4)$$

Here,

$$a' = a + \frac{\sum_d L_d N_d}{2},$$

$$b' = b + \frac{1}{2} \sum_{d=1}^D \sum_{n=1}^{N_d} k(\mathbf{x}_{dn}, \mathbf{x}_{dn}) - \frac{1}{2} \sum_{j=1}^Q \mu_j^\top \Lambda_j^{-1} \mu_j, \quad (5)$$

and

$$\mu_j = \Lambda_j \sum_{d=1}^D \sum_{n: s_{dn}=j} \hat{\mathbf{k}}_d, \quad \Lambda_j^{-1} = \sum_{d=1}^D N_{dj} \hat{\mathbf{K}}_d + r\mathbf{I}. \quad (6)$$

where  $\hat{\mathbf{k}}_d$  represents the kernel evaluated in the  $\mathbf{x}_{dn}$  objects that has the cluster assignment  $j$ ,  $\hat{\mathbf{K}}_d$  is the Gramm matrix of the projection matrices for each domain  $d$ , and  $N_{dj}$  is the number of shape descriptors assigned to cluster  $j$  in the brain structure  $d$  (domain).

The posterior for the precision parameter  $\alpha$  is given by

$$p(\alpha|\Phi, \mathbf{S}, \mathbf{W}, a, b) = \mathcal{G}(a', b'), \quad (7)$$

and the posterior for the latent vector  $\zeta_j$  is given by

$$p(\zeta_j|\alpha, \Phi, \mathbf{S}, \mathbf{W}, r) = \mathcal{N}(\mu_j, \alpha^{-1} \Lambda_j). \quad (8)$$

### 2.3. Inference

In order to marginalize out the latent vectors  $\mathbf{Z}$ , and the precision parameter  $\alpha$ , we use stochastic EM algorithm [10]. To this end, collapsed Gibbs sampling for the cluster assignments  $\mathbf{S}$ , and maximum joint likelihood estimation of the projection matrices  $\mathbf{W}$  are alternately iterated.

In the E-step, a new value for  $s_{dn}$  is sampled from

$$p(s_{dn} = j|\Phi, \mathbf{S}_{\setminus dn}, \mathbf{W}, a, b, r, \gamma) \propto \frac{p(s_{dn} = j, \mathbf{S}_{\setminus dn}|\gamma)}{(\mathbf{S}_{\setminus dn}|\gamma)} \times \frac{p(\Phi|s_{dn} = j, \mathbf{S}_{\setminus dn}, \mathbf{W}, a, b, r)}{p(\Phi_{\setminus dn}|\mathbf{S}_{\setminus dn}, \mathbf{W}, a, b, r)}, \quad (9)$$

where  $\setminus dn$  represents a value excluding the  $n$ th descriptor in the  $d$ th shape (domain). The first factor in the expression above is given by

$$\frac{p(s_{dn} = j, \mathbf{S}_{\setminus dn}|\gamma)}{p(\mathbf{S}_{\setminus dn}|\gamma)} = \begin{cases} \frac{N_{\cdot j \setminus dn}}{N - 1 + \gamma} & \text{for an existing cluster} \\ \frac{\gamma}{N - 1 + \gamma} & \text{for a new cluster.} \end{cases} \quad (10)$$

In the M-step, the projection matrices  $\mathbf{W}$  are estimated by maximizing the logarithm of the joint likelihood (2). The gradient of the joint likelihood is computed by

$$\frac{\partial \log p(\Phi, \mathbf{S}|\mathbf{W}, a, b, r, \gamma)}{\partial \mathbf{W}_d} = \times \left[ \left( -N_{dj} \Lambda_j \frac{\partial \hat{\mathbf{K}}_d}{\partial \mathbf{W}_d} \Lambda_j \right)^\top \times \sum_{e=1}^D \sum_{n: s_{dn}=j} \hat{\mathbf{k}}_d + \Lambda_j^\top \sum_{n: s_{dn}=j} \partial \hat{\mathbf{k}}_d \right] - \frac{1}{2} \sum_{j=1}^Q N_{dj} \text{Tr} \left( \frac{\partial \hat{\mathbf{K}}_d}{\partial \mathbf{W}_d} \Lambda_j \right). \quad (11)$$

## 3. RESULTS

## 4. CONCLUSIONS

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## 5. REFERENCES

- [1] D. Aiger, N. J. Mitra, and D. Cohen-Or. 4-points congruent sets for robust surface registration. *ACM Transactions on Graphics*, 27(3):#85, 1–10, 2008.
- [2] Alexander M. Bronstein, Michael M. Bronstein, Leonidas J. Guibas, and Maks Ovsjanikov. Shape google: Geometric words and expressions for invariant shape retrieval. *ACM Trans. Graph.*, 30(1):1:1–1:20, February 2011.
- [3] Michael M. Bronstein and Iasonas Kokkinos. Scale-invariant kernel signatures for non-rigid shape recognition. In *In Proc. CVPR*, 2010.
- [4] Alan Brunton, Augusto Salazar, Timo Bolkart, and Stefanie Wuhler. Review of statistical shape spaces for 3d data with comparative analysis for human faces. *Computer Vision and Image Understanding*, 128(0):1 – 17, 2014.
- [5] Xavier Cortés and Francesc Serratosa. An interactive method for the image alignment problem based on partially supervised correspondence. *Expert Syst. Appl.*, 42(1):179–192, 2015.
- [6] A. Cosa, S. Canals, A. Valles-Lluch, and D. Moratal. Unsupervised segmentation of brain regions with similar microstructural properties: Application to alcoholism. In *Engineering in Medicine and Biology Society (EMBC), 2013 35th Annual International Conference of the IEEE*, pages 1053–1056, July 2013.
- [7] S. Durrleman, T Fletcher, G. Gerig, and M Niethammer, editors. *Spatio-temporal Image Analysis for Longitudinal and Time-Series Image Data*, volume 8682. Springer, 2014.
- [8] Derek Hill. Neuroimaging to assess safety and efficacy of ad therapies. *Expert Opinion on Investigational Drugs*, 19(1):23–26, 2010. PMID: 19947893.
- [9] Tomoharu Iwata, Tsutomu Hirao, and Naonori Ueda. Unsupervised cluster matching via probabilistic latent variable models, 2013.
- [10] Tomoharu Iwata, Tsutomu Hirao, and Naonori Ueda. Probabilistic latent variable models for unsupervised many-to-many object matching. *Information Processing and Management*, 52(4):682 – 697, 2016.
- [11] Arto Klami. Variational bayesian matching. In *Proceedings of the 4th Asian Conference on Machine Learning, ACML 2012, Singapore, Singapore, November 4-6, 2012*, pages 205–220, 2012.
- [12] Arto Klami, Seppo Virtanen, and Samuel Kaski. Bayesian canonical correlation analysis. *J. Mach. Learn. Res.*, 14(1):965–1003, April 2013.
- [13] Luming Liang, Andrzej Szymczak, and Mingqiang Wei. Geodesic spin contour for partial near-isometric matching. *Computers & Graphics*, 46:156–171, 2015.
- [14] Dongdong Lin, Vince D. Calhoun, and Yu-Ping Wang. Correspondence between fmri and SNP data by group sparse canonical correlation analysis. *Medical Image Analysis*, 18(6):891–902, 2014.
- [15] K. A. Sidorov, S. Richmond, and D. Marshall. Efficient groupwise non-rigid registration of textured surfaces. In *Proceedings of the 2011 IEEE Conference on Computer Vision and Pattern Recognition, CVPR '11*, pages 2401–2408, Washington, DC, USA, 2011. IEEE Computer Society.
- [16] Bharath K. Sriperumbudur, Arthur Gretton, Kenji Fukumizu, Bernhard Schölkopf, and Gert R.G. Lanckriet. Hilbert space embeddings and metrics on probability measures. *J. Mach. Learn. Res.*, 11:1517–1561, August 2010.
- [17] Paul M. Thompson, Kiralee M. Hayashi, Greig de Zubicaray, Andrew L. Janke, Stephen E. Rose, James Semple, David Herman, Michael S. Hong, Stephanie S. Dittmer, David M. Doddrell, and Arthur W. Toga. Dynamics of gray matter loss in alzheimer’s disease. *The Journal of Neuroscience*, 23(3):994–1005, 2003.
- [18] Oliver van Kaick, Andrea Tagliasacchi, Oana Sidi, Hao Zhang, Daniel Cohen-Or, Lior Wolf, , and Ghasan Hamarneh. Prior knowledge for part correspondence. *Computer Graphics Forum (Proc. Eurographics)*, 30(2):553–562, 2011.
- [19] Xu Yang, Hong Qiao, and Zhi-Yong Liu. Partial correspondence based on subgraph matching. *Neurocomputing*, 122:193 – 197, 2013. Advances in cognitive and ubiquitous computing Selected papers from the Sixth International Conference on Innovative Mobile and Internet Services in Ubiquitous Computing (IMIS-2012).