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Enhancing Diffusion MRI Measures By Integrating Grey and White Matter Morphometry With Hyperbolic Wasserstein Distance

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Abstract

In order to improve the preclinical diagnose of Alzheimer's disease (AD), there is a great deal of interest in analyzing the AD related brain structural changes with magnetic resonance image (MRI) analyses. As the major features, variation of the structural connectivity and the cortical surface morphometry provide different views of structural changes to determine whether AD is present on presymptomatic patients. However, the large scale tensor-valued information and relatively low imaging resolution in diffusion MRI (dMRI) have created huge challenges for analysis. In this paper, we propose a novel framework that improves dMRI analysis power by fusing cortical surface morphometry features from structural MRI (sMRI). We first compute the hyperbolic harmonic maps between cortical surfaces with the landmark constraints thus to precisely evaluate surface tensor-based morphometry. Meanwhile, the graph-based analysis of structural connectivity derived from dMRI is conducted. Next, we fuse these two features via the optimal mass transportation (OMT) and eventually the Wasserstein distance (WD) based single image index is computed as a potential clinical multimodality imaging score. We apply our framework to brain images of 20 AD patients and 20 matched healthy controls, randomly chosen from the Alzheimer's Disease Neuroimaging Initiative (AD-NI2) dataset. Our preliminary experimental results of group classification outperformed those of some other single dMRI-based features, such as regional hippocampal volume, mean scores of fractional anisotropy (FA) and mean axial (MD). The novel image fusion pipeline and simple imaging score of structural changes may benefit the preclinical AD and AD prevention research.

Index Terms

Alzheimer's Disease; Wasserstein Distance; Graph Laplacian; Fusion; Morphometry

1. Introduction

Many neurodegenerative diseases have been found to come with the brain anatomical changes, for instance, Alzheimer's disease (AD) [1]. By observing the disease related structural alterations, it might help physicians to precisely diagnose patients even at the

preclinical stage. Diffusion MRI (dMRI) is a powerful technique to study white matter structures such as the fiber connection that reflect axonal organization. However, its large scale tensor-valued information and relatively low imaging resolution (2-3 mm) have created huge challenges for analysis. Because of the noise and partial volume effects, there are frequent false-negative and false-positive results [2]. In recent years, there is a growing interest to take a multi-model analysis approach to improve dMRI image analysis power [3, 4]. On the other hand, in clinical settings, one would favor a single imaging score [5], which capitalizes on as much of the data in the image as possible. Naturally, a stable method to compute a single imaging index by integrating features from both sMRI and dMRI would be highly advantageous to this research field.

Wasserstein distance (WD), also known as the earth mover's distance, evaluates the similarity of two distributions under the optimal mass transportation [6]. It measures the minimal amount of the work needed to move the total mass contained in one distribution onto another. The WD has been widely used in computer vision studies to model shape variances and image mapping [7, 8]. For instance, Su et al. combined the conformal geometry and optimal mass transportation theory to construct a novel conformal Wasserstein shape space [9]. In our previous research [10], we applied the WD to measure cortical surface morphometrical difference in the hyperbolic space where brain surfaces were modeled by high-genus surfaces when six biologically meaningful landmarks were regarded as surface boundaries. In this paper, we propose a novel dMRI analysis framework with the goal to verify the consistency/inconsistency of structural variations between different modalities by hyperbolic WD.

Our work is driven by the idea that there are possible relations between anatomical features captured by different modalities, e.g. dMRI and T1 sMRI. It is worth noting that the organization of fiber connections to some extent affects the shape of brain surface [11] and AD progression may correlate with these two types of features separately [12, 13]. We want to evaluate whether the Wasserstein distance, which represents the minimal transport costs between two feature spaces constructed from these two different imaging data, is able to provide a concise imaging descriptor for the relationship. Specifically, features extracted from the grey/white matter surface, e.g. tensor-based morphometry, and the structural connectivity map drawn by fiber probability tractography are fused by the hyperbolic WD and used for AD diagnosis. The main contributions of our paper are: (1) we propose a novel computational model to integrate anatomical features of grey and white matter; (2) we generalize the WD research to empower dMRI study by defining a single clinical multimodality imaging score which is informative to summarize the underlying brain structure changes. Our preliminary experimental results show good promise to improve the efficiency and efficacy of dMRI analysis for clinical research.

2. Methods

2.1. Subjects and Data Acquisition

The data used in this study comes from ADNI2 project [14] and we randomly pick 20 subjects for each diagnose group, i.e. AD and normal controls. The participants of ADNI2 project underwent the whole brain MRI scanning on 3T GE Medical Systems scanners.

Standard anatomical T1-weighted SPGR (spoiled gradient echo) sequences were collected by following parameters: 256×256 matrix; voxel size = $1.2 \times 1.0 \times 1.0 \text{ mm}^3$; TI = 400 ms; TR = 6.98 ms; TE = 2.85 ms; flip angle = 11° . Moreover, diffusion-weighted images (DWI) were acquired as: 256×256 matrix; voxel size: $2.7 \times 2.7 \times 2.7 \text{ mm}^3$; TR = 9000 ms; scan time = 9 min; 46 separate images were acquired for each dMRI scan: 5 T2-weighted images with no diffusion sensitization (b0 images) and 41 diffusion-weighted images ($b = 1000 \text{ s/mm}^2$). More details about image acquisition can be found at http://adni.loni.usc.edu/wp-content/uploads/2010/05/adni2_mri_training_manual_final.pdf.

2.2. dMRI-based Brain Connectivity Network Feature

Let us first describe the procedure of parameterization of brain structural network with the reference of inter-regional fiber connectivity. The probabilistic fiber tracking is performed in standard space using FSL software package [15], where each pair of brain regions calculate 5000 times of probability tractography and number of traces that reach both source and target regions is regarded as the structural connection between them. Given the a weighted adjacent matrix $A_{n \times n} = \{a_{ij}, i, j < n\}$, a_{ij} represents the probabilistic fiber connection between region i and region j ; n is the number of brain regions depended on the chosen brain atlas (Desikan-Killiany Atlas [16]) (here $n = 34$). We then calculate the correlation matrix of A and take the absolute value, denoted as R , which measures similarity of the probability fiber connection patterns between each pair of the brain regions. For each individual, R matrix is treated as the brain connectivity network. Elements of R range from 0 to 1 whose value closer to 1 means stronger relation. After that, we constructed the weighted Laplacian $L = D - R$, where $D(i)$ is called the degree matrix, defined as:

$$D(i, j) = \begin{cases} \sum_{j=1}^n R_{ij} & \text{if } i=j, \\ 0 & \text{, otherwise.} \end{cases} \quad (1)$$

Based on the spectral graph theory, the eigenvector corresponding to lower order of eigenvalue of the Laplacian matrix contains the ‘low frequency’ information [17], i.e. the latent structure of connectivity networks. We pick the smallest order p such that, for all subjects, the p -th smallest eigenvalue are larger than 0. The eigenvector corresponding to the p -th smallest eigenvalue is regarded as the descriptor of the individual connectivity schemes. Given a template and a source subject, their connectivity descriptors are

$V_t = \{V_t^i, i=1, \dots, n\}$ and $V_s = \{V_s^i, i=1, \dots, n\}$ respectively, we measure the difference of structural connectivity between them as $V = \{e^{V_s^i - V_t^i}, i=1, \dots, n\}$.

2.3. Surface Tensor-based Morphometry Feature

Given a surface S embedded in R^3 with Riemannian metric g as $\{S, g\}$, if there is another metric on S , $\bar{g} = e^{2u}g$, then $\bar{g}$ is a conformal deformation of g , i.e. has the same angle measures as g , and u is the conformal factor. There are infinite conformal deformations to a given $\{S, g\}$. Among them, the uniformization theorem guarantees that a unique representative which induces constant Gaussian curvature everywhere. The constant will be one of $\{-1, 0, 1\}$ and the corresponding metric is called the uniformization metric of S . In

this paper, we embed the universal covering space of the studied brain surface to the hyperbolic space H^2 which is suitable for high-genus surfaces with negative Euler numbers. The uniformization metric of such embedding is computed by the surface Ricci flow [18]. The normalized Ricci flow is defined as $dg(t)/dt = (4\pi\chi(S)/A(0) - 2K(t))g(t)$, where $\chi(S)$ is the Euler characteristic of S which is related to the total Gaussian curvature $\int_S K dA$. $A(0)$ is the total area of S at time 0. It has been proved that when $\chi(S) < 0$, the solution of the above equation exists for all $t > 0$ and converges to a metric with constant Gaussian curvature -1 everywhere [19].

With the hyperbolic uniformization metric, we can isometrically embed the surface onto the Poincare disk (Fig 1, B(2)) and further convert it to the Klein model. The hyperbolic lines in

the Klein model coincide with Euclidean lines by such a transformation $Z \rightarrow \frac{2Z}{1+Z\bar{Z}}$. Next we should build the initial map between surfaces via the constrained harmonic map. Given a surface $\{S, g\}$, if the coordinates (x, y) satisfy $g = e^{2u(x, y)}(dx^2 + dy^2)$, u is the conformal factor, (x, y) are called the isothermal coordinates. Suppose there is a map f between two surface $f: \{S_1, g_1\} \rightarrow \{S_2, g_2\}$, we denote $f(z) = w$, $z \in S_1$, $z = x + iy$ and $w \in S_2$, $w = u + iv$. z, w are the local isothermal coordinates respectively. The harmonic energy of the map f is defined as

$$E(f) = \int_{S_1} \rho(f(z))(|f_z|^2 + |f_{\bar{z}}|^2) dx dy \quad (2)$$

where $g_1 = \sigma(z) dz d\bar{z}$ and $g_2 = \rho(w) dw d\bar{w}$, $f_z = \frac{1}{2}(\frac{\partial f}{\partial x} - i\frac{\partial f}{\partial y})$, $f_{\bar{z}} = \frac{1}{2}(\frac{\partial f}{\partial x} + i\frac{\partial f}{\partial y})$. The map that at the critical point of the harmonic energy is called the harmonic map. By solving the

Euler-Lagrange equation $f_z \bar{z} + \frac{\rho w}{\rho} w_z w \bar{z} \equiv 0$ and meanwhile adding alignment of the corresponding boundaries of the paired Klein polygons as boundary condition which accomplished by linear interpolation through the arc length parameter, we can constructed the initial map. Due to the convexity of the target domain, the planar harmonic maps are guaranteed to be diffeomorphic.

The hyperbolic metric of the cortical surface requires to be decomposed to several hyperbolic polygons before computing the initial mapping. The inter-subject pair-wise constrained harmonic mappings of polygons are then glued together to form a global homeomorphism (Fig1, B(4)). This mapping need to be improved via non-linear heat diffusion which will eventually achieve a global hyperbolic harmonic map. Suppose $f: M \rightarrow N$ is the initial map, it can be expressed as $f(z) = w$ locally. The diffusion process is given by the following gradient descent method

$$\frac{df(z, t)}{dt} = [s_z \bar{z} + \frac{\rho_w(w)}{\rho(w)} f_z f_{\bar{z}}] \quad (3)$$

where $\rho(w) = \frac{1}{(1 - w\bar{w})^2}$ is the hyperbolic metric in the Poincare disk.

The surface tensor-based morphometry (TBM) can be computed based on the hyperbolic harmonic mapping f . The derivative map of f is the linear map between the tangent spaces $df: TM(p) \rightarrow TM(f(p))$, which defined the Jacobian matrix of f . With triangular meshes, the derivative map df is approximated by the linear map from one face $[v_i, v_j, v_k]$ to another $[w_i, w_j, w_k]$. Both v_i and w_i are embedded on the Poincare disk. The Jacobian matrix of the map can be point-wise discretized as $J = df = [w_3 - w_1, w_2 - w_1] [v_3 - v_1, v_2 - v_1]^{-1}$. The TBM is defined as $\sqrt{\det(j)}$, which measures the amount of local area changes induced by map f and has been widely used in the previous morphometric research [20, 21].

2.4. Wasserstein Distance

The Wasserstein distance (WD) measures the cost of the optimal mass transportation map (OMT) between two probability measures. In this research, we use the WD to quantify the relation between cortical surface morphometry and structural connectivity encoded by the eigenvector of the graph Laplacian of fiber connectivity matrix. First, we define the power Voronoi diagram in the following way. Given a point set P and its corresponding weight vector w , the power Voronoi diagram induced by (P, w) is a cell decomposition of the surface (P, g) , such that the cell spanned by a set of discrete initial center points on S , p_i is given by

$$\text{Cell}_i = \left\{ x \in S \mid d_g^2(x, p_i) - w_i \leq d_g^2(x, p_j) - w_j \right\}, i \neq j. \quad (4)$$

$d_g(x, p_i)$ is the geodesic distance between x and p_i in hyperbolic space. The surface-based OMT map can be computed by the power Voronoi diagram and it further induces the WD. Given a Riemannian manifold (S, g) , μ and ν represent two probability measures defined on S and they have the same total mass. ν is a Dirac measure with discrete point set support $P = \{p_1, p_2, \dots, p_n\}$ and $\nu(p_i) = v_i$. Then there exists a weight vector $w = \{w_1, w_2, \dots, w_n\}$, unique up to a constant, such that the power Voronoi diagram induced by (P, w) gives the OMT map between μ and ν as $\phi: \text{Cell}_i \rightarrow p_i, i = 1, 2, \dots, n$ and satisfied $\int_{\text{Cell}_i} \mu(x) dx = v_i, \forall i \in [1, 2, \dots, n]$. The optimal weight can be computed and updated repeatedly in the direction

$$\frac{dw_i}{dt} = v_i - \int_{\text{Cell}_i} \mu(x) dx, x \in S. \quad (5)$$

Here, vertex-wise probability μ is defined as TBM value while the Dirac measure ν is the structural connectivity difference. With the hyperbolic metric, the hyperbolic WD between two measures is defined as:

$$WD(\mu, \nu) = \sum_{i=1}^n \int_{\text{Cell}_i} (\tanh^{-1} |\frac{x - p_i}{1 - x \bar{p}_i}|)^2 \mu(x) dx \quad (6)$$

3. Experimental Results

Each individual cortical surface is reconstructed by using Freesurfer software [22] and we only use the left hemisphere in our experiment as previous research showed that AD related brain atrophy may start from left side and gradually extends to the right [23]. Six landmarks are automatically traced via Caret software [24] that are found biologically meaningful and stable to brain development and degeneration [24]. All the results of surface reconstruction and landmark delineation are visually inspected. After being cut along the six landmarks, cortical surfaces become multiply connected surfaces. It helps set landmarks as the boundary constraint to guide accurate surface mappings, a technique frequently used in our prior work [25]. After cortical surfaces are parameterized with discrete hyperbolic Ricci flow, we randomly pick up one subject as the template and register the remaining cortical surfaces to it with the hyperbolic harmonic mapping which is diffeomorphic everywhere. The Jacobian matrix of the mapping is computed and eventually we get the vertex-wise surface TBM. For connectivity feature, after computing the satisfied eigenvector of Laplacian matrix, which measures the similarity of fiber connectivity patterns between each pair of brain regions, we set it as the Dirac values of template. The elements of the eigenvectors are assigned to the centroid vertex of the brain regions which, in our method, are defined according to the Desikan-Killiany Atlas. The optimal mass transportation map from surface feature to connectivity feature is optimized via gradient descent and the WD is computed in the hyperbolic space. We show several OMT results with the power Voronoi diagram in the Fig 2, B&C.

With the computed WD, we apply the simple tree classifier [26] to classify them into two groups and compare the result with the diagnosis type. The classification accuracy of the multi-model WD with 5-fold cross validation is 77.5%. By contrast, we also compute other two standard disease related features via dMRI images, e.g. fractional anisotropy (FA) and mean diffusivity (MD). FA is a summary measure of microstructural integrity while MD is an inverse measure of membrane density that sensitive to cellularity, edema and necrosis. We use their mean values as single image scores and the same classifier is applied with 5-fold cross validation. We summarize the results in the Table 1. The results show that the proposed WD outperform the other two statistics in our experiment. Moreover, we compare our proposed feature with the regional disease sensitive index, hippocampal (HP) volume. Interestingly, WD shows more powerful detection of AD than HP volume.

4. Conclusion and Future Work

In this paper, we proposed a novel method that fuses the two structural features. One feature describes the regional fiber connectivity patterns over the whole brain that computed from dMRI images and the other measures the cortical surface morphometry based on the hyperbolic harmonic mapping. We adapted the hyperbolic WD to evaluate the similarity and

dissimilarity of those two measures after conducting the optimal mass transportation over the probability distribution maps. The classification result using hyperbolic WD suggests our method, compared to other dMRI single features, to be a potential way to help the AD diagnosis and prevention.

The current work represents our first step toward achieving an automatic single brain imaging system to integrate sMRI and dMRI data. There are several potential opportunities to further improve our work. For example, the brain atlas might influence the organization of OMT maps. Future work could focus on the vertex-wise dMRI connectivity patterns instead of regional-wise schemes by using high resolution dMRI data. Besides, the probability measures for the surface-based morphometry may be replaced with other measures, e.g. cortical thickness or multivariate features, in order to become fully informative to the shape variances.

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Fig. 1.

Pipeline showing the fusion of white and grey matter features. Panel A shows the raw datasets, dMRI and T1 images. Panel B shows surface tensor-based morphometry analysis, (1) surface reconstruction by Freesurfer and landmark tracing by Caret; (2) the parameterized surface on hyperbolic domain; (3) universal covering space of (1) in the Poincaré disk model; (4) Hyperbolic pants decomposition for harmonic mapping. Panel C shows (1) brain structural connectivity networks, left hemisphere only, with 34 subregions; (2) connectivity matrix, which measures the similarity of fiber connectivity of each pair of subregions. Panel D illustrates the optimal mass transportation between TBM and properties of structural networks, shown as the hyperbolic power Voronoi diagram.

Fig. 2.

In panel A, six landmarks automatically traced are treated as the boundary constraints for hyperbolic harmonic mapping. SF, sylvian fissure; aSTG, anterior half of the superior temporal gyrus; CeS, central sulcus; CaS, calcarine sulcus; MWdS, media wall dorsal segment; MWvS, medial wall ventral segment. Panel B, C show three AD and control samples, respectively, after evaluating the OMT map and presented as the hyperbolic power Voronoi diagram.

Table 1
Classification on different measures

Method	Classification Accuracy	False Positive Rate
WD	77.5%	24%
FA	47.5%	57%
MD	70.0%	27%
HP Volume	74.5%	25%

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