A Geometric Analysis of ODFs As Oriented Surfaces for Interpolation, Averaging and Denoising in HARDI Data

Sentibaleng Ncube  
Florida State University  
sentibaleng@hotmail.com

Sentibaleng Ncube  
Florida State University  
qxie@stat.fsu.edu

Anuj Srivastava  
Florida State University  
asrivastava@fsu.edu

Abstract

We propose a Riemannian framework for analyzing orientation distribution functions (ODFs), or corresponding probability density functions (PDFs), in HARDI for use in comparing, interpolating, averaging, and denoising. Recent approaches based on the Fisher-Rao Riemannian metric result in geodesic paths that have limited biological interpretations. As an alternative, we develop a framework where we separate the shape and orientation features of PDFs, compute geodesics under their respective Riemannian metrics and then combine them to form a pseudo-geodesic on the product space. These pseudo-geodesic paths have better biological interpretation (in terms of interpolating points between given PDFs by preserving shape diffusivity and anisotropy) and provide tools for pairwise comparing and averaging a collection of PDFs. The latter tools, in turn, are useful for interpolation, denoising, and improved tractography HARDI. We demonstrate these ideas using both synthetic and real HARDI data.

1. Introduction

The diffusion tensor MRI (DT-MRI) data has been used for studying brain structures, their connectivities, and functionalities consisting of fields of diffusion-tensor matrices in the imaged volume. The problems involving denoising, interpolation, tractography, and related analyses for such data require a framework for comparing, averaging, and manipulating these tensor structures. For example, a simple idea for denoising the diffusion tensor at any voxel is to take a weighted average of tensors at its neighboring voxels. Since the space of diffusion tensors, the set of $3 \times 3$ positive-definite symmetric matrices, is a nonlinear manifold, these tasks are naturally performed in a Riemannian framework. Several past papers have presented such Riemannian frameworks for the analysis of diffusion tensors and their usages in data analysis and tractography [10, 15, 9].

In recent years, the increased strengths of MRI scanners have led to the possibility of measuring diffusion orientations beyond the three canonical directions, and have led to HARDI (High Angular Resolution Diffusion Imaging) technology that measures fluid flow at each voxel in numerous directions [18]. The basic unit of HARDI data at each anatomical location is an orientation diffusion function (ODF) that captures the diffusivity as a function of the direction. In principle, one obtains the diffusivity values for all directions although, in practice, these values are collected only for a small subset of directions. Using smooth interpolations, e.g. using spherical harmonics, one can obtain an ODF on the full sphere. From those limited observations, an ODF can be viewed as a non-negative function on $S^2$. The space of ODFs is, thus, the set of all such functions on $S^2$. We would like to pursue a Riemannian framework for analyzing ODFs, similar to past frameworks for analyzing diffusion tensors. However, since this space is quite different from the set of diffusion tensors, the earlier methods do not naturally extend to HARDI data and new ideas are needed. A major difference in HARDI data, from the DTI data, is that the ODFs are functions, and this function space is an infinite-dimensional space.

We start with the question: What Riemannian structures are suitable for analyzing HARDI data? Keep in mind that an important use of HARDI data (or ODF fields) is in tractography, i.e. the task of discovering major fluid pathways in the human brain using orientations of ODFs. Let $f : S^1 \to \mathbb{R}^+$ denote an ODF, and let $\mathcal{F}$ be the set of all such square-integrable ODFs. Any ODF has three specific properties of interest: (i) direction(s) of diffusivity or orientation(s), (ii) diffusivity pattern or shape, and (iii) global magnitude of diffusivity or scale. By analyzing the elements of $\mathcal{F}$, one directly works with these three features – orientation, shape, and scale – and their relative contributions in the analysis are as dictated by the chosen metric. Many researchers tend to focus on the shape and orientations of the ODFs by removing the scale variability. They do so by forming the corresponding probability density functions (PDFs), $g(s) = f(s)/\int_{S^2} f(s) ds$. For example, Mcgraw et al. [13] model the PDF at each voxel as a mixture of von Mises-Fisher parametric densities. The space of all PDFs, call it $\mathcal{P}$, is a Banach manifold, and it can become a Hilbert manifold by choosing a Riemannian structure. So far, there have been two main choices of Riemannian metrics for $\mathcal{P}$. (These metrics also apply to $\mathcal{F}$ in a similar way, but we will describe them only for $\mathcal{P}$.)

The first idea is to use the standard $L^2$ metric and the
geodesic distances are given by the $L^2$ norms of the differences, i.e. $d(f_1, f_2) = \| f_1 - f_2 \|$. Surprisingly, despite its simplicity, very few past papers have actually used this metric for HARDI data analysis. The other idea, that has become increasingly popular in recent years, is to use the Fisher-Rao Riemannian metric. This metric was introduced by Rao [16], for comparing populations using the Fisher information matrix but, recently, the nonparametric version of the Fisher-Rao metric has become prominent for studying PDFs [17]. The use of the Fisher-Rao metric in HARDI data analysis was first proposed in Chang et al. [7], and later described in several other papers, including [11, 6]. It must be noted that very few papers have compared or justified the usage of the Fisher-Rao metric over the $L^2$ metric. It is well-known that the Fisher-Rao metric allows the re-parameterizations of functions via isometries, but none of the papers in HARDI data analysis have utilized re-parameterizations of PDFs.

In this paper, we highlight a major disadvantage of using either the $L^2$ metric or the Fisher-Rao metric directly. The main problem lies in the fact that in a direct formulation, the shape and the orientation features get mixed and, as a result, the geodesic paths between PDFs go through PDFs that are not amenable to biological interpretations. Instead, we used a square-root representation under which the Fisher-Rao metric reduces to the standard $L^2$ metric. In this scheme, a PDF $g \in \mathcal{P}$ is represented by its positive square-root $h(s) = \frac{g(s)}{\sqrt{g(s)}}$; this function is also called a half-density function (HDF). An HDF has the property that its $L^2$ norm is: $\int_{S^2} h(s)^2 ds = \int_{S^2} g(s) ds = 1$. Therefore, the space of all such half-densities, call it $\mathcal{H}$, is a subset of the unit Hilbert sphere in $L^2$.

Since $\mathcal{H}$ is a unit sphere, the geodesic distance between any points, under the $L^2$ metric, is simply the length of the shortest arc connecting them: $d_h(h_1, h_2) = \cos^{-1}(\int_{S^2} h_1(s)h_2(s) ds)$. Furthermore, the geodesic path between any two points can be written analytically as:
\[
\psi_h(t) = \frac{1}{\sin(d_h)} \left[ \sin(d_h(1-t))h_1 + \sin(td_h)h_2 \right].
\]

This geodesic has been used for interpolation and imputation of missing data between ODFs in several papers [7, 11, 6]. A statistical analysis on a manifold often involves the tangent bundle of a manifold, since the tangent spaces are vector spaces that allow more conventional statistics. To enable mappings between the manifold $\mathcal{H}$, and its tangent space at a point $h$, $T_h(\mathcal{H})$, one uses the exponential map and its inverse, given by:
\[
\exp_h(w_h) = \cos(t \parallel w_h \parallel)h_1 + \sin(t \parallel w_h \parallel) \frac{w_h}{\|w_h\|},
\]
\[
\exp_h^{-1}(h_2) = \frac{d_h}{\sin(d_h)}(h_2 - \cos(d_h)h_1).
\]

Using these expressions, one can compute the Karcher mean of PDFs, under the Fisher-Rao metric. For a collection of PDFs, $p_1, p_2, \ldots, p_n$, represented by their HDFs $h_1, h_2, \ldots, h_n$, their Karcher mean is defined to be the HDF that minimizes the sum of the squared distances: $\mu_h = \arg \min_{h \in \mathcal{H}} \sum_{i=1}^n d_h(h, h_i)^2$. The algorithm for computing the Karcher mean has become standard in the literature and is not elaborated here. Roughly speaking, it is an iterative process that evaluates the gradient of the cost function given above, using the exponential map and its inverse, and updates the estimate of $\mu_h$, using this gradient until convergence.

Although the Fisher-Rao Riemannian framework is very convenient for the analysis of HARDI data, the results obtained are not always meaningful in biological terms. We illustrate this problem with a 2D example, where one is interested in analyzing PDFs on $S^1$. (With a slight abuse of
Figure 2: Geodesic interpolations of PDFs in $\mathcal{H}$ (top) and $\mathcal{G}$ (bottom).

Figure 3: Karcher mean of PDFs in different spaces.

Note that unlike discrete entropy, differential entropy can be negative. Therefore it is possible to get an FA greater than 1.

Figure 1: Geodesic path between PDFs in $\mathcal{H}$ (top) and $\mathcal{G}$ (bottom).

FA=.4754 .3670 .3076 .3719 .6031 .8775
FA=.4754 .5944 .3540 1.1888 .8907
FA=.5944 .3540 1.1888 .8907
FA=.5944 .3540 1.1888 .8907
FA=.5944 .3540 1.1888 .8907
FA=.5944 .3540 1.1888 .8907

3. Proposed Riemannian Framework

The main idea is to separate shape and orientation features in PDFs and treat them as separate variables. We impose Riemannian metrics on the shape and orientation spaces, construct geodesic paths in these spaces, and then combine them appropriately to form pseudo-geodesics between given PDFs. The separation of shape and orientation is accomplished by using the algebraic quotient operation, as described next.

3.1. Shape Analysis of PDFs

We consider a PDF $g$, on a unit sphere $S^2$, as a surface in $\mathbb{R}^3$. In other words, we analyze the full graph of $g$, rather than the function $g$ itself. All references to a PDF (HDF), hereafter, imply the underlying surface associated with the graph of that PDF (HDF). Since an element $h \in \mathcal{H}$ is a surface in $\mathbb{R}^3$, the rotation group $SO(3)$ acts on it by rigid rotation around the origin of $S^2$: $SO(3) \times \mathcal{H} \to \mathcal{H}$ given by $(O,h) = Oh$. We define an equivalence relation on $\mathcal{H}$, by setting any two HDFs to be equivalent, if they are within a rotation of each other, i.e. for any two $h_1, h_2 \in \mathcal{H}$, we have $h_1 \sim h_2$ if $h_2 = (O,h_1)$ for some $O \in SO(3)$. An equivalence class is given by the orbit of an element under $SO(3)$, $[h] = \{(O,h) | O \in SO(3)\}$. The set of all equivalence classes is given by $\mathcal{S} = \{[h] | h \in \mathcal{H}\} = \mathcal{H}/SO(3)$, which is the quotient space of $\mathcal{H}$ under the action of $SO(3)$.

The space, $\mathcal{S}$, provides a natural way to quantify dissimilarities between shapes of PDFs on $S^2$, while ignoring their orientations and, hence, is referred to as the shape space of PDFs. Since the action of $SO(3)$ on $\mathcal{H}$ is by isometries, under the Fisher-Rao metric on $\mathcal{H}$, we can inherit the resulting distance on $\mathcal{S}$ and obtain:

$$d_s([h_1],[h_2]) = \min_{O \in SO(3)} d_h(h_1,(O,h_2)).$$

This implies that we keep $h_1$ fixed and find the optimal rotation of $h_2$ that minimizes the geodesic distance between them. Note that $d_s$ is a proper distance which satisfies all three properties of a distance. We have implemented a gradient-based approach for solving the optimization problem on $SO(3)$. (The 2D case, shown for illustration, requiring optimization over $S^1$, can be performed efficiently.
the pseudo geodesic in $G$}

Comparing the Karcher means obtained in (column 1-4), while each of the densities are rotationally aligned. Since the orientation information of fiber tracts is important in tractography, we cannot simply discard this information.

Similarly, the Karcher mean of PDFs in the quotient space $S$, is the HDF that minimizes the sum of squared distances: $\mu_s = \arg\min_{h \in G} \sum_{i=1}^{n} d_s([h], [h_i])^2$. In fig.3, column 6, we compute the mean shape for same collection of HDFs (column 1-4), while each of the densities are rotationally aligned. Comparing the Karcher means obtained in $H$ and $S$, we see there is a much clearer interpretation for the shape in $S$.

### 3.2. Joint Quotient and Orientation Space

Since the orientation information of fiber tracts is important in tractography, we cannot simply discard this information. Instead, we form a product space between the quotient $S$ and the orientation $SO(3)$ that results in an eventual PDF representation space $G = S \times SO(3)$. An element in $g \in G$ has two components: shape $[h] \in S$ and orientation $O \in SO(3)$ (relative to a fixed PDF). However, rather than using their product geometry, we will consider a different combination as follows.

The differential geometry of $SO(3)$ under Euclidean metric is quite standard and is not repeated. We will use $d_s(O_1, O_2) = ||\log(O_1^T O_2)||/\sqrt{2}$ as the geodesic distance between any two elements of $SO(3)$. For any two elements $g_1, g_2 \in G$, we will construct a pseudo-geodesic path in $G$.

First we construct a geodesic path between their shape components $[h_1]$ and $[h_2]$ in $S$ and a geodesic path between their orientation components $O_1$ and $O_2$ in $SO(3)$. Then, we combine the two paths to form a composite pseudo geodesic in $G$ (Fig.4), according to:

$$\hat{h}_2(t) = \exp(t \log(O^*)) ;$$

where $\hat{h}_2(t) = \exp(t \log(O^*)), h_2)$.

In other words, we take the shape function at the $t^{th}$ time,
Figure 6: Interpolation of PDFs on a square grid, given the four corner PDFs. The left result is for Fisher-Rao metric on $P$, while the right result is on the joint shape-orientation space $S \times SO(2)$. Executed by assuming diffusion begins at a seed point usually given at the boundary of a square grid. From this seed point, a fiber tract is assumed to propagate in the direction of maximum diffusion within the voxel. When the voxel boundary is reached, the tract then travels in the direction dictated by the ensuing voxel. In our experiments, we introduce seed points at the bottom (or side) of a square grid. In these experiments, we use unimodal densities with clear orientations (i.e. high diffusivity in a certain direction). If we consider the interpolation results using the Fisher-Rao metric, shown in the left columns of Figs.6 and 7, the intermediate shapes are often bimodal and lack clear orientations. One can imagine using such interpolations for tractography applications, where we expect the results will not be of good quality. Despite having narrow unimodal densities (denoting clear tract orientations) at the corner, the tract orientations at the intermediate voxels are ambiguous. In contrast, the results from interpolations in $G$ are much more structured. Not only are the intermediate PDFs unimodal, but also their orientation is consistent with the direction of the given (corner) PDFs. This is due to the modified formulation that preserves the shape and orientation structures as much as possible.

Now we present some results using real HARDI data. Here Diffusion Weighted Magnetic Weighted Images (DW-MRI) are used to generate ODFs in HARDI data sets. The DWI data was provided by UCLA Laboratory of Neuro Imaging. In the data set, 30 images were acquired: 3 with no diffusion sensitization (i.e. T2-weighted images) and 27 diffusion-weighted images in which the gradient directions were evenly distributed on the hemisphere. The reconstruction matrix was 128x128, yielding a 1.8x1.8 mm$^2$ in-plane resolution. The ODFs were reconstructed from the data using a Cartesian Tensor basis method developed in [2, 3]. Fig. 8 displays a region of interest (ROI) in an MRI slice.

Figure 7: Interpolation of PDFs on a square grid, given the four corner PDFs, using weighted Karcher means in $H$ (left) and $G$ (right).

Figure 8: Selected Regions of Interest for HARDI Data (left) and in the ODF field (right) contained in the ROI in the left.

As in the first experiment, we take two PDFs corresponding to few voxel separation and interpolate between them using geodesics in $H$ and pseudo-geodesics in $G$, and compare them with the actual PDFs in those intermediate voxels. The first example is shown in Fig.9 where the top path is the actual path, the middle path is the geodesic path in $H$ and the third path is the pseudo-geodesic in $G$. As observed in the simulated data experiments, the pseudo-geodesic in $G$ better preserves the shape and anisotropy of the intermediate PDFs.

Now we apply our framework grid interpolation using real PDFs. The goal of this experiment is to extract a square region of real HARDI data, then compare it to the interpolated field of PDFs in $H$ and $G$ respectively, given the four corner PDFs (in blue-green). Fig. 10 shows the ROI in the MRI slice and the corresponding ODF field. In the middle row we show the actual PDF field and in the bottom row we show the estimated ODF field using only the corner ODFs. Though we are no longer dealing with unimodal densities, it is clear to see that in $G$ the shape is preserved, and the orientation transitions in a very smooth, gradual way. Contrary to $G$, the interpolation in $H$ is very distorted in some parts.
Actual Path

Geodesic Path in Representation Space, $\mathcal{H}$

Pseudo-Geodesic Path in Joint Shape-Orientation Space, $\mathcal{G}$

Figure 9: Interpolating paths in HARDI Data Set

ROI in MRI Slice

ROI in ODF Field

Interpolation in $\mathcal{H}$

Interpolation in $\mathcal{G}$

Figure 10: Interpolation of HARDI Data Field on a square grid when compared to the actual data field given. For example, in the top row of the interpolated field in the representation space, we see the shape becoming distorted, as two bumps are being created in different locations in that part of the grid. The orientation is also affected since the bumps may not be in the proper locations.

5. Conclusion

We have presented a modification of the Fisher-Rao framework for analyzing PDFs in HARDI data. This method is based on separating the shape and orientation of PDFs, and analyzing them using their individual Riemannian framework. The resulting pseudo-geodesic is found to better preserve shape, anisotropy and other physical properties, when compared to the direct Fisher-Rao geodesic.

References