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by

L.J. Astola, A. Fuster, L.M.J. Florack

Centre for Analysis, Scientific computing and Applications
Department of Mathematics and Computer Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven, The Netherlands
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A Riemannian Scalar Measure for Diffusion Tensor Images

Laura Astola^a, Andrea Fuster^b, Luc Florack^a

^a*Department of Mathematics and Computer Science, Eindhoven University of Technology, Den Dolech 2, 5600 MB Eindhoven, The Netherlands*

^b*Department of Biomedical Engineering, Eindhoven University of Technology, Den Dolech 2, 5600 MB Eindhoven, The Netherlands*

Abstract

We study a well-known scalar quantity in Riemannian geometry, the Ricci scalar, in the context of Diffusion Tensor Imaging (DTI), which is an emerging non-invasive medical imaging modality. We derive a physical interpretation for the Ricci scalar and explore experimentally its significance in DTI. We also extend the definition of the Ricci scalar to the case of High Angular Resolution Diffusion Imaging (HARDI) using Finsler geometry. We mention that Ricci scalar is not only suitable for tensor valued image analysis, but it can be computed for any mapping $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ ($m \leq n$), for example when an original image changes in time.

Keywords: Riemann Geometry, Diffusion Tensor Imaging, Ricci Scalar, Finsler geometry, High Angular Resolution Diffusion Imaging

1. Introduction

Diffusion Tensor Imaging (DTI) is a non-invasive magnetic resonance imaging technique that measures the intra-voxel incoherent motion of water molecules in tissue [1, 2]. Here we focus on its applications to study the brain white matter. In this context, DTI is being used in clinical research, for example to localize major white matter tracts in the vicinity of tumors, thus assisting in surgical planning. DTI also enables the assessment of white matter maturation in preterm infants. At each voxel, the information from Diffusion Weighted Imaging (DWI) measurements is stored in a so-called diffusion tensor, which can be represented by a 3×3 symmetric and positive definite matrix. One can construct different types of scalars based on these

diffusion tensors. Although a tensor contains more information than a scalar, scalar measures are indispensable for their simplicity and unambiguity.

Indeed several scalar measures have been proposed in the DTI-literature. Typically they capture certain features of the tensor valued image, giving some insight into the underlying tissue structure. This in turn can indicate the presence of white matter-related pathologies. The most popular scalar measures are the mean diffusivity (MD) and the fractional anisotropy (FA) [3].

In this paper we consider a well-known scalar quantity in Riemannian geometry, the Ricci scalar, in the analysis of DTI-images. In 2D image processing the Ricci scalar has been used for curvature analysis [4]. The goal of this research is to evaluate whether the Ricci scalar can provide additional information on white matter structures compared to the established scalar measures. We also extend this measure beyond DTI, to high angular resolution diffusion imaging (HARDI), a framework which has certain advantages over DTI. We found promising preliminary results on simulated and phantom data showing negative values of the Ricci scalar at voxels with crossing structures.

This paper is organized as follows. In Section 2, we derive the metric tensors that are essential for computing curvatures from the DTI-data, and show the definition of the Ricci scalar in detail. In Section 3 we give an intuitive physical interpretation of this scalar measure and include a pseudo-code for the computation. Section 4 contains a brief survey of the popular scalar measures in DTI up to this date. In Section 5 we show results from several experiments using simulated, phantom and real DTI data. In Section 6 we take an extended definition of Ricci scalar for Finsler spaces and connect this to HARDI via higher (than second) order tensors. Finally in Section 7 we draw some conclusions and discuss the direction of future work.

2. Theory

In human tissue the random thermal motion of water molecules is restricted by the surrounding micro structures. Therefore the range of displacement of an average particle can have a directional bias. In DTI a second order model is assumed and this range is determined by the diffusion tensor

D . This tensor D can be computed from a collection of signals S_i from measurements that are sensitive to molecular displacements in spatial direction $\mathbf{v}_\alpha$, using the following Stejskal-Tanner equation

$$S_\alpha = S_0 \exp(-b \cdot \mathbf{v}_\alpha^T D \mathbf{v}_\alpha) , \quad \alpha = 1, 2, 3 . \quad (1)$$

where S_0 is the non-weighted signal and b a known scalar. Because of the positivity of the measurements and their symmetry w.r.t. the origin, D is a symmetric, positive definite second-order tensor in dimension three. The physical unit of diffusion is m^2/s and so we must assign the inverted unit s/m^2 to the inverse $g = D^{-1}$ of the diffusion tensor. In this way we have encoded to the tensor g , the information of the average time needed for particles to diffuse in certain directions. Thus g can be seen as a metric tensor [5, 6] with large diffusion in a certain direction corresponding to a short distance in the metric space. Such a tensor defines the inner products, i.e. the position dependent lengths and angles in the image that are induced by the diffusion. A number of authors have incorporated tools from Riemannian geometry in the analysis of diffusion tensor images [7, 8, 9, 10, 11, 12].

We use the Einstein's summation convention, meaning that whenever the same Latin index appears in subscript and superscript, a sum is taken over them as in the following example:

$$a_i u^i := \sum_i a_i u^i . \quad (2)$$

While in Euclidean space with standard cartesian coordinates, an inner product of two vectors v, w is

$$\langle v, w \rangle = \delta_{ij} v^i w^j , \quad (3)$$

where δ_{ij} denotes the (components) of the identity matrix, on the tangent space of a Riemann manifold the inner product of two tangent vectors v, w is

$$\langle v, w \rangle = g_{ij} v^i w^j , \quad (4)$$

and is thus determined by the metric tensor g_{ij} . The explicit schemes to compute the so-called covariant derivative and the Riemann curvature, which we will use in the following, are in the Appendix.

Since we have a metric tensor $g = D^{-1}$, i.e. an inner product $\langle, \rangle_g$ defined at each image voxel we can compute Riemannian curvatures. The Riemann curvature vector is

$$R(X, Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z , \quad (5)$$

where $\nabla_V U$ is the covariant derivative [6] of U in direction V and

$$[U, V] = U^i \frac{\partial}{\partial x^i}(V) - V^i \frac{\partial}{\partial x^i}(U) . \quad (6)$$

It is a measure of the non-commutativity of the covariant derivative. In a Euclidean space $R(X, Y)Z = 0$ for all $X, Y, Z \in \mathbb{R}^n$. Having defined the Riemann curvature vector, we can compute the so-called sectional curvature with respect to a plane determined by two non-collinear vectors X, Y

$$\langle R(X, Y)X, Y \rangle := g_{ij}(R(X, Y)X)^i Y^j , \quad (7)$$

which is an inner product of curvature vector and one of its input vectors. In dimension two, this is actually the Gaussian curvature [13]. By choosing a vector V , and taking the average of the sectional curvature w.r.t. every plane that contains vector V , we obtain the Ricci curvature in direction V , which indicates whether the geodesic with initial points in a small neighborhood of a given point p , with initial direction V , tend to merge towards or diverge away from the geodesic that goes through p with tangent vector V [10]. This Ricci curvature can be computed as follows:

$$Ric_p(V) = \sum_{X_i \perp V} \langle R(X_i, V)X_i, V \rangle , \quad (8)$$

where X_i spans the orthonormal basis $V^\perp$. Finally, by taking the sum of the Ricci curvatures in every spatial direction we end up with the Ricci scalar

$$R = \sum_{\alpha} Ric(V_{\alpha}) , \quad (9)$$

where V_{α} , $\alpha = 1, 2$ span an orthonormal basis. Alternatively, one can compute the Ricci scalar simply as

$$R = g^{ik} g^{jl} \langle R(U_i, U_j)U_k, U_l \rangle , \quad (10)$$

where for example in 3D (which is the dimension of interest here) by choosing the standard orthonormal basis $U_1 = X$, $U_2 = Y$, and $U_3 = Z$. Details on how to compute this are in the Appendix.

Unlike the metric, the Ricci tensor is not positive definite, allowing for both positive and negative values of the Ricci scalar. This is a major difference with respect to the usual DTI scalar measures, which are typically positive. In dimension three the Ricci scalar does not completely characterize the curvature but represents instead the average of the characterizing curvatures.

3. Interpretation

The Ricci scalar is a so-called intrinsic curvature, meaning that it is not measured using concepts as the radii of osculating circles, that refer to the ambient Euclidean space that contains the manifold itself. It measures how much the volume of a small ball on the manifold differs from the volume of a small Euclidean ball with the same radius. For example, given an initial point on a surface, we can compute the geodesics of unit length with all possible initial directions. By connecting the end points, we obtain a closed curve, whose length depends on the Ricci scalar of the surface. For illustration see Fig. 1. Say, we consider the monkey saddle surface in Fig. 1 as a "warped"

Figure 1: Left: A surface with positive Ricci scalar. Middle: A surface with Ricci scalar zero. Right: A surface with everywhere non-positive Ricci scalar.

or distorted $\mathbb{R}^2$, i.e. flat plane. We can compute the metric tensors and visualize the corresponding ellipsoids that quantify the distortion in x - and y -directions as in Fig. 2. We see that in those areas, where neighboring tensors have different orientations the Ricci scalar is negative. This is what we expect to happen also in higher dimensions. Ricci scalar would be then a natural indicator of inhomogeneities of tensors. In diffusion tensor imaging, such inhomogeneities can correspond to crossing/passing fiber bundles.

4. Scalar Measures in DTI

We briefly review the literature on scalar measures in diffusion tensor image analysis. Let λ_1, λ_2 and λ_3 be the eigenvalues of the diffusion tensor

Figure 2: Left: The ellipsoids describing the metric tensors on the original domain. Right: Ricci scalars on the original domain.

D . In [14], the trace

$$\text{tr}(D) = \lambda_1 + \lambda_2 + \lambda_3 , \quad (11)$$

and anisotropy indices

$$\lambda_1/\lambda_2 , \quad \lambda_1/\lambda_3 , \quad \lambda_2/\lambda_3 , \quad (12)$$

were introduced in the context of DTI. The mean diffusivity (MD) is defined as

$$\hat{\lambda} = \text{tr}(D)/3 , \quad (13)$$

and it measures the average amount of diffusion in a voxel. The fractional anisotropy (FA) [3] is defined as

$$\text{FA} = \sqrt{\frac{3}{2}} \frac{\sqrt{(\lambda_1 - \hat{\lambda})^2 + (\lambda_2 - \hat{\lambda})^2 + (\lambda_3 - \hat{\lambda})^2}}{\sqrt{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}} . \quad (14)$$

The FA of an isotropic tensor is zero, and for a tensor with nonzero first eigenvalue and approximately vanishing second and third eigenvalues, the

FA approaches value 1. If we represent the diffusion tensor with an ellipsoid, with semi-axes as the eigenvectors with lengths proportional to eigenvalues, this means that a sphere has FA zero and an elongated cigar-shaped ellipsoid has FA close to one. See Figure 3 for an illustration of the differences between FA and the Ricci scalar.

Figure 3: From left to right: a homogeneous isotropic tensor field $R = \text{FA} = 0$, a homogeneous anisotropic field $R = 0$, $\text{FA} \neq 0$, an inhomogeneous isotropic field $R \neq 0$, $\text{FA} = 0$, and an inhomogeneous anisotropic field $R \neq 0$, $\text{FA} \neq 0$.

As in [3], one can decompose a diffusion tensor into its isotropic and anisotropic part. In [3], this decomposition is done by solving the eigenvalues, but alternatively this can be done as follows. If we denote the isotropic and anisotropic parts of a matrix M as M_I and M_A respectively then

$$M_I = \frac{1}{3} \begin{pmatrix} M_{11} + M_{22} + M_{33} & 0 & 0 \\ 0 & M_{11} + M_{22} + M_{33} & 0 \\ 0 & 0 & M_{11} + M_{22} + M_{33} \end{pmatrix}, \quad (15)$$

and

$$M_A = \frac{1}{3} \begin{pmatrix} 2M_{11} - M_{22} - M_{33} & M_{12} & M_{13} \\ M_{12} & 2M_{22} - M_{11} - M_{33} & M_{23} \\ M_{13} & M_{23} & 2M_{33} - M_{11} - M_{22} \end{pmatrix}. \quad (16)$$

The relative anisotropy (RA) [3] is the ratio

$$\text{RA} = \frac{|M_A|_F}{|M_I|_F}, \quad (17)$$

where $|\cdot|_F$ denotes the Frobenius matrix norm. On the other hand, defining these quantities using eigenvalues makes it obvious that these are all

rotational invariants and do not depend on the choice of an orthonormal coordinate system. Another measure introduced in the early years of DTI is the volume ratio (VR) [15]

$$VR = \frac{\lambda_1 \lambda_2 \lambda_3}{(\hat{\lambda})^3} . \quad (18)$$

In Fig. 4, we have plotted a surface that is swept by all possible tuples of $(\lambda_1, \lambda_2, \lambda_3)$ for which $\lambda_1 + \lambda_2 + \lambda_3 = c$ (i.e. the first octant of a regular sphere), with samples of magnitudes of the VR and the FA. Some additional invariant

Figure 4: Left: The lengths of the blue arrows represent the magnitude of the VR corresponding to triple of eigenvalues $(\lambda_1, \lambda_2, \lambda_3)$. Right: As on the left hand side, but with the lengths corresponding to the FA. Indeed the FA is largest when one of the eigenvalues is large compared to the others and the VR is largest when all eigenvalues are equal.

scalar measures that are derived from the previous have been proposed in [16]. While FA and MD are the most popular scalar measures in clinical research, in [17, 18] plotting the FA in the region of interest (ROI) on a $(|M_I|_F, |M_A|_F)$ -plane is seen to be useful.

So far, all the scalars in this section have been pointwise measures, that is they contain information only on the diffusion tensor in a particular voxel.

One of the first measures that gather information also from the neighborhood of a particular voxel is the lattice index (LI) [19, 20]. For example when the diffusion is isotropic, the eigenvectors of neighboring tensors have no correlation. On the other hand, it is reasonable to expect that in case of coherently organized tissue, (at least at a sufficient resolution) there will be such a correlation. Let us denote the componentwise product of two tensors A and B as $\langle A, B \rangle_F$, a reference tensor as M and a neighboring tensor as M^α , then a basic LI is

$$LI = \sqrt{\frac{3}{8}} \left(\frac{\sqrt{\langle M_I, M_I^\alpha \rangle}}{\sqrt{\langle M, M^\alpha \rangle}} + \frac{(\sqrt{\langle M_I, M_I^\alpha \rangle})^2}{\langle M, M \rangle} \right). \quad (19)$$

By weighting LI's with the inverse of voxel distance a local contextual anisotropy measure can be computed in any ROI w.r.t. the reference voxel [20]. Based on LI, another lattice index measure which is more robust to noise has been proposed in [21]. In one of the first proposals to use Riemannian geometry [10] to produce differential scalar measures for DTI, it is suggested to take the inner product between the eigenvector of the diffusion tensor and the most coherent direction of local diffusion i.e. the eigenvector of the Ricci tensor that corresponds to the greatest eigenvalue. This measures the degree to which the principal eigenvector determined by a single tensor is aligned with the locally most coherent direction. By this direction we mean the direction along which the neighboring geodesics, which are the analogues of straight lines in the curved space distorted by anisotropic diffusion, tend to stick together. In DTI fiber tracking and segmentation it is necessary to use the information on the neighboring tensors. Ricci scalar is a mean curvature measure and as such takes the whole neighborhood into account. The diameter of the neighborhood can be tuned by a proper scale selection for the derivative operator [22].

5. Experiments

In order to explore the geometric significance of the Ricci scalar, we have experimented with simulated, physical phantom and real data.

5.1. Simulated Data

To get insight in what the Ricci scalar can detect in a tensor field, we refer to Fig. 5, where we have simulated a crossing of oriented sets of tensors,

modeling homogeneous diffusion tensors corresponding to two fiber bundles. In the center of the crossing region of this tensor field, the Ricci scalar tends to be negative. Since the Ricci scalar involves second order derivatives (see Appendix), the minimum size of the region to be considered depends on the scale of the Gaussian differential operator [22, 23].

Figure 5: Left: A simulated crossing of tensors. Middle: Ellipsoids representing the diffusion profiles on the image slice in the middle of crossing. Right: A temperature map (blue is negative and red is positive) of the Ricci scalars on the previous plane. In the middle of the crossing we obtained negative values, also when we varied the angle of crossing.

5.2. Phantom Data

We computed Ricci scalars on a real phantom consisting of cylinder containing a water solution, three sets of crossing synthetic fiber bundles and three supporting pillars on the boundary. In Fig. 6 we see that in the region close to the crossing bundles Ricci scalars have relatively large negative values, despite the noisy nature of the DTI-data. Due to the resolution, we did not obtain exactly same results as with the simulated data, which is more ideal representation of a crossing structure.

Figure 6: Top left: A physical phantom, with three crossings. Top right: A mean of HARDI images from the top of the cylinder on the left. Middle left: Diffusion tensors in the foremost crossing area, marked by yellow dashed lines, solid line estimating the lateral center of the crossing. Middle right: Ricci scalars in "temperature map" corresponding to previous area. Blue (red) means negative (positive). Bottom left: Diffusion tensors slightly off the plane that includes the crossing. Bottom right: Ricci scalars on the same slice. A planar picture can not fully show the three dimensional situation. Physical phantom by courtesy of Pim Pullens.

5.3. Real Data

We have also experimented with real DTI data of a rat brain. We plotted the Ricci scalars in a temperature map, to emphasize the differences in sign. We identified positive (negative) outliers of the Ricci scalar data with maximum (minimum) values of the rest of the data. The Ricci scalar gives information about the local spatial variations in diffusion tensor orientations unlike FA, which will identify tensors with similar anisotropy even if their orientations differ. This can be seen e.g. in the boxed region in Fig. 7, which is known to have complex structure [24].

Figure 7: Left: Ricci scalars on a slice of the rat brain DTI image. Middle: Fractional anisotropy. Right: Mean diffusivity.

6. Ricci Scalar for High Angular Resolution Diffusion Imaging

In the previous we considered the Ricci scalar in Riemannian geometry. In DTI, we see from the expression $\mathbf{v}_i^T D\mathbf{v}_i$ in Eq. (1) that the diffusion profile (a spherical surface with diffusion constant as the radius) is a second order polynomial on the sphere. This model is insufficient in voxels that contain two or more bundles of axonal fibers with different orientation. To be able to model more complex shapes of diffusion profiles, we use Finsler geometry [25, 26, 27, 28, 29, 30], which is a general framework that also includes Riemann geometry as a special case. Instead of DTI, we consider high angular resolution diffusion images (HARDI) [31] that contain more angular measurements than the DTI, although it is possible to use (typically up to 6th order) Finsler-model also on DTI. In Riemannian space, to each point we can associate a second order metric tensor. In Finsler space we can associate a convex norm function to each point. First question is how to construct

such a convex function from a HARDI measurement. For this we compute the so-called orientation distribution function (ODF) [32] that represents the actual diffusivity profile. Then, all we need to do is to convexify this profile. This can be done for example as suggested in [28], or by representing the diffusion profile as an n th order polynomial and then taking a n th root as suggested in [30]. Whatever the method, as soon as we have a (strongly) convex [25] modification of the spherical diffusion profile, we can compute directional metric tensors $g_{ij}(y)$ that locally approximate the profile [26, 30]. Let $F(x, y)$ be the convex function, where $x = (x^1, x^2, x^3)$ stands for spatial direction and $y = (y^1, y^2, y^3)$ the unit tangent vector originating from x . Then the directional metric tensor g_{ij} is computed as follows

$$g_{ij} = \frac{1}{2} \frac{\partial^2 F(x, y)}{\partial y^i \partial y^j} . \quad (20)$$

The Ricci curvature can be then computed in a similar manner to the Riemannian case, keeping in mind that the tangent vector y is fixed. The Ricci scalar $Ric(x, y)$ becomes then [26]

$$Ric(x, y) = R_i^i(y) , \quad (21)$$

where

$$R_k^i(x, y) = 2 \frac{\partial G^i(x, y)}{\partial x^k} - y^j \frac{\partial^2 G^i(x, y)}{\partial x^j \partial y^k} + 2 G^i(x, y) \frac{\partial^2 G^i(x, y)}{\partial y^j \partial y^k} - \frac{\partial G^i(x, y)}{\partial y^j} \frac{\partial G^j(x, y)}{\partial y^k} . \quad (22)$$

The G here is the so-called geodesic coefficient [26]

$$G^i(x, y) = \frac{1}{4} g^{il}(x, y) \left(2 \frac{\partial g_{jl}(x, y)}{\partial x^k} - \frac{\partial g_{jk}(x, y)}{\partial x^l} \right) y^j y^k . \quad (23)$$

A drawback is that the formulae become more complicated and that the interpretation becomes more difficult due to the y -dependence.

7. Discussion and Outlook

Besides in fiber tracking the Ricci scalar may be useful in voxel classification. After the classification, the regions with single orientation are identified as the regular DTI data (second order tensors), and higher order models (e.g. fourth order tensors) can be used in regions where inhomogeneous fiber population is anticipated. It is clear that the Ricci scalar does

not give information on the shape of the individual tensors, but of the second order change w.r.t. the surrounding tensors. It could also be useful in the so-called splitting tracking method in HARDI framework [33], by indicating the potential bifurcation points of fiber bundles with large negative values. It goes without saying that DT-MRI images are not the only possible applications, although they are especially suitable simply because the metric tensors come with the data "for free". The physical interpretation of the generalized Ricci scalar as well as its practical applications to the analysis of HARDI data is an interesting problem for future research.

8. Appendix

To compute Riemannian Ricci scalars, we essentially need only to know the diffusion tensors and Riemann tensors. The necessary ingredients are then the diffusion tensors and their componentwise differentials up to order two. It may be convenient to compute the Riemann tensors using Christoffel symbols γ_{ij}^k :

$$\gamma_{ij}^k = \frac{1}{2} g^{kl} \left(\frac{\partial g_{il}}{\partial x^j} + \frac{\partial g_{jl}}{\partial x^i} - \frac{\partial g_{ij}}{\partial x^l} \right), \quad (24)$$

where $g^{ij}g_{jk} = \delta_k^i$. The components of the Riemann tensor can be defined as

$$\begin{aligned} R_{ijks} &= \langle R(X^i, X^j)X^k, K^s \rangle \\ &= g_{ms} \left(\gamma_{ik}^l \gamma_{jl}^m + \frac{\partial}{\partial x^j} \gamma_{ik}^m - \gamma_{jk}^l \gamma_{il}^m - \frac{\partial}{\partial x^i} \gamma_{jk}^m \right), \end{aligned} \quad (25)$$

where X^l span the orthonormal basis on the tangent space. We computed the necessary derivatives by applying Gaussian derivatives to the whole tensor volumes, storing the results, and then taking the linear combinations indicated in Eq. (24) and (25). What may look like a tedious task is really only book-keeping and fortunately in 3D there are only six independent components of the Riemann tensor. Although the expressions will get longer, we may also use the fact that we can express the components of Riemann tensor in terms of sectional curvatures [34], and there are essentially only three of these in 3D.

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