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Fourth-order tensor invariants in high angular resolution diffusion imaging

by

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Fourth-order Tensor Invariants in High Angular Resolution Diffusion Imaging

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\textbf{Abstract.} We consider new scalar quantities in the context of High Angular Resolution Diffusion Imaging (HARDI), namely, the principal invariants of fourth-order tensors modeling the diffusion profiles. We present the formalism needed to compute tensor invariants. We show results on the orthogonal basis of fourth-order tensor and on real HARDI phantom and brain data.

1 Introduction

Diffusion MRI is a magnetic resonance imaging technique that measures the rate of water diffusion in biological tissue. It is widely used to study brain white matter in a non-invasive way. The diffusion tensor is a second-order tensor constructed from diffusion data which can reveal information on the white matter architecture. This model is called diffusion tensor imaging (DTI). However, this approach fails in the case of complex configurations of white matter fiber bundles, such as crossings. A new diffusion MRI acquisition scheme has been proposed to overcome this difficulty: High Angular Resolution Diffusion Imaging (HARDI) \cite{1}, in which the diffusion correlated signal decay is measured in a large number of directions.

The visualization and interpretation of HARDI data is complex and challenging. Meaningful scalar quantities constructed from the data are therefore desirable, in particular in view of future clinical application of HARDI. Scalar measures are used to characterize tissue anisotropy and distinguish between single or multi-fiber white matter configurations, for example. A number of HARDI scalar quantities have been suggested so far, such as generalized anisotropy (GA) and scaled entropy (SE) \cite{2} and generalized fractional anisotropy (GFA) \cite{1}.

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In this paper we propose the use of (higher-order) tensor invariants as building blocks for scalar measures in the analysis of HARDI images. Tensor invariants are scalar quantities constructed from the tensor which are independent of the coordinate system used to express the tensor components. Invariants of the second-order diffusion tensor have been studied in [3, 4]. The most widely used anisotropy measure in DTI, fractional anisotropy (FA), is in fact an invariant of the diffusion tensor. Invariants of a fourth-order covariance tensor have been considered in DTI [5] and for the diffusion kurtosis tensor in [6], with a different definition of the eigenvalues needed to compute invariants. In this paper invariants of fourth-order tensors are studied for the first time in the context of HARDI. The paper is organized as follows. We first describe the modeling of HARDI data by higher-order tensors and how to compute invariants in the fourth-order case. We perform experiments on an orthogonal basis of fourth-order tensors as well as tensors corresponding to real HARDI phantom and brain data, and discuss the results and possibilities for further work.

2 Theory

2.1 Modeling of HARDI data by tensors

The orientation distribution function (ODF) constructed from raw HARDI data describes the diffusivities per direction in a voxel. Algorithms converting the raw data to an ODF or a so-called solid angle ODF can be found, for example, in [7, 8]. An ODF can be approximated by a higher-order (> 2) 3-dimensional tensor [9]:

\[ D(g) = D_{i_1...i_n}g^{i_1}...g^{i_n} \]  

where \( g = (g^1, g^2, g^3) \) is a direction on the unit sphere and \( n \) is the order of the tensor. Here we use the Einstein summation convention for repeated indices. Tensor \( D \) represents a generalized diffusion tensor, and as such, only even orders \( n = 2k (k = 1, 2, \ldots) \) are considered. In addition, these tensors are fully symmetric. In this paper we consider the case where HARDI data is modeled by fourth-order tensors.

2.2 Eigenvalues of a fourth-order tensor

It is not straightforward to generalize the notion of eigenvalues to tensors of order higher than two. A number of authors have addressed this issue for both symmetric and non-symmetric tensors [10–14]. A possible approach to determine the eigenvalues and eigentensors of a fourth-order tensor \( T \) is the following [5, 6, 15, 16]

\[ T : X = \lambda X \]

where \( X \) is a second-order eigentensor and \( \lambda \) is the associated eigenvalue. Such eigenvalues are sometimes called Kelvin eigenvalues. The tensor double dot product is defined as

\[ T : X = T_{ijkl}X_{kl} \]
where indices run from 1 to \( d \), the dimension of the tensor (in our case \( d = 3 \)).

We can also write (2) as

\[
(T_{ijkl} - \lambda I_{ijkl}) X_{kl} = 0
\] (4)

Here, \( I_{ijkl} = \delta_{ik}\delta_{jl} \) is the fourth-order identity tensor. This equation has an eigentensor \( X \neq 0 \) as a solution if the following characteristic equation is satisfied:

\[
\det (T - \lambda I) = 0
\] (5)

Note that this formulation holds for arbitrary fourth-order tensors, and independently of the symmetries possessed by the tensor. In practice we can solve the eigenvalue problem (2) by considering the second-order embedding of \( T \) as shown in the next section.

### 2.3 Matrix representation

An arbitrary 3-dimensional fourth-order tensor \( T \) has 81 independent components and can therefore be represented by a \( 9 \times 9 \) matrix. On the other hand, a 3-dimensional fourth-order tensor \( D \) satisfying the major and minor symmetries

\[
D_{ijkl} = D_{klij} = D_{jikl} = D_{ijlk}
\] (6)

has only 21 independent components. Such a tensor can be mapped to a 6-dimensional second-order tensor \( \tilde{D} \) represented by a symmetric \( 6 \times 6 \) matrix [5, 17]. Requiring also that \( D_{ijkl} = D_{ikjl} \) we have the full symmetry leading to 15 independent components and e.g. the following matrix representation for \( \tilde{D} \):

\[
\tilde{D} = \begin{pmatrix}
D_{1111} & D_{1122} & D_{1133} & \sqrt{2}D_{1112} & \sqrt{2}D_{1113} & \sqrt{2}D_{1123} \\
D_{1122} & D_{2222} & D_{2233} & \sqrt{2}D_{1222} & \sqrt{2}D_{1233} & \sqrt{2}D_{2233} \\
D_{1133} & D_{2233} & D_{3333} & \sqrt{2}D_{1333} & \sqrt{2}D_{1323} & \sqrt{2}D_{2333} \\
\sqrt{2}D_{1112} & \sqrt{2}D_{1122} & \sqrt{2}D_{1133} & 2D_{1112} & 2D_{1122} & 2D_{1133} \\
\sqrt{2}D_{1113} & \sqrt{2}D_{1223} & \sqrt{2}D_{1233} & 2D_{1123} & 2D_{1223} & 2D_{1233} \\
\sqrt{2}D_{1123} & \sqrt{2}D_{2223} & \sqrt{2}D_{2233} & 2D_{1133} & 2D_{1233} & 2D_{2233}
\end{pmatrix}
\] (7)

The factors of 2 and \( \sqrt{2} \) guarantee that \( \tilde{D} \) transforms as a second-order tensor. On the other hand, (7) has 6 real eigenvalues \((\lambda_1, \ldots, \lambda_6)\) since it is a (real) symmetric \( 6 \times 6 \) matrix. In fact, the eigenvalues of the fourth-order tensor \( D \) and the eigenvalues of \( \tilde{D} \) are the same [5, 6, 16].

### 2.4 Principal invariants

The principal invariants of a fourth-order tensor arise as coefficients of the characteristic equation (5). In the case of a fully symmetric fourth-order tensor this equation has six roots or eigenvalues and therefore there are six principal invariants \( I_1, \ldots, I_6 \):

\[
\lambda^6 - I_1 \lambda^5 + I_2 \lambda^4 - I_3 \lambda^3 + I_4 \lambda^2 - I_5 \lambda + I_6 = 0
\] (8)
The principal invariants of the fully symmetric fourth-order tensor $D$ can be calculated in terms of its six eigenvalues as follows \([5, 16, 18]\):

\[
I_1 = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 \\
I_2 = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \ldots + \lambda_5\lambda_6 \\
I_3 = \lambda_1\lambda_2\lambda_3 + \lambda_1\lambda_2\lambda_4 + \ldots + \lambda_4\lambda_5\lambda_6 \\
I_4 = \lambda_1\lambda_2\lambda_3\lambda_4 + \lambda_1\lambda_2\lambda_3\lambda_5 + \ldots + \lambda_3\lambda_4\lambda_5\lambda_6 \\
I_5 = \lambda_1\lambda_2\lambda_3\lambda_4\lambda_5 + \ldots + \lambda_2\lambda_3\lambda_4\lambda_5\lambda_6 \\
I_6 = \lambda_1\lambda_2\lambda_3\lambda_4\lambda_5\lambda_6
\] (9)

Here, $I_1 = \text{trace } D$ and $I_6 = \text{det } D$. Note that in principle the invariants and eigenvalues can take on both positive and negative values. This is not in conflict with the tensor being positive definite, as it should be for a tensor characterizing diffusion. In the case of higher-order tensors positive eigenvalues are a sufficient but not necessary condition for positive definiteness \([14]\).

3 Experiments

We compute the principal invariants of fourth-order tensors corresponding to a basis of real spherical harmonics and to HARDI data of a phantom representing a crossing of two fiber bundles. We also perform experiments on real brain data of a 25 year old healthy volunteer.

3.1 Real spherical harmonics

An alternative to the tensor model is to use a basis of real spherical harmonics (SH) $\tilde{Y}_l^m$ \([9, 19]\):

\[
\tilde{Y}_l^m = \begin{cases} 
\sqrt{2} \text{ Re } Y_l^m & \text{if } m < 0 \\
\text{ Re } \frac{1}{\sqrt{2}} Y_l^0 & \text{if } m = 0 \\
\sqrt{2} \text{ Im } Y_l^m & \text{if } m > 0 
\end{cases}
\] (10)

Here $Y_l^m$ are the usual complex spherical harmonics. A fourth-order fully symmetric diffusion tensor can be expressed in terms of the 15 real spherical harmonics with $l = 0, 2$ and $l = 4$. The glyphs of the different components are given in Figure 1, where an isotropic tensor is added to simulate realistic DOT/Q-ball ODF. Subsequently, we consider the fourth-order tensor equivalent to each of the SH’s and compute its eigenvalues and principal invariants. Results are given in Tables 1, 2 and 3.

We notice a number of interesting patterns arising in the invariants of the considered orthogonal basis. First of all, many SH modes share the same or very similar invariants, as it should be for SH’s represented by glyphs with the same or a comparable shape. Invariants corresponding to SH’s with $l = 2$ are all equal, except for the $m = 0$ mode. Invariants of SH’s with $l = 4, m \neq 0$ are also very similar. As a rule, invariants of $\tilde{Y}_l^m$ and $\tilde{Y}_l^{-m}$ are the same, for $l, m \neq 0$. We also note that $I_2$ is the same for all SH’s with fixed $l$, independent of the value
of $m$. On the other hand, it is not straightforward to identify particular glyph shapes from a given set of invariant values. Another feature is that invariants of SH’s with $m = 0$ are all different from zero, independent of the value of $l$. Such modes represent isotropic diffusion for $l = 0$ or anisotropic diffusion in a single direction for $l = 2, 4$ (see Figure 1). On the other hand, the only non-zero invariants of SH’s with $m \neq 0$ are $I_2$ and $I_4$ (and just $I_2$ for $m = \pm 4$). However, the values of these invariants for $l = 4$ are relatively large compared to those of $l = 2$, especially in the case of $I_4$. This might be helpful in order to distinguish between regions where diffusion data is well described by a second-order tensor (DTI) and regions where a higher-order model is needed (HARDI).

![Real spherical harmonics. Top row: $\tilde{Y}_0^0$. Middle row: $\tilde{Y}_2^{-2}, \tilde{Y}_2^{-1}, \tilde{Y}_2^0, \tilde{Y}_2^1, \tilde{Y}_2^2$. Bottom row: $\tilde{Y}_4^{-4}, \tilde{Y}_4^{-3}, \tilde{Y}_4^{-2}, \tilde{Y}_4^{-1}, \tilde{Y}_4^0, \tilde{Y}_4, \tilde{Y}_4^2, \tilde{Y}_4^4$.](image)

**Table 1.** Invariants corresponding to SH’s with $l = 0$.

<table>
<thead>
<tr>
<th>$l = 0$</th>
<th>$(I_1, \ldots, I_6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_0^0$</td>
<td>{1.4103, 0.7955, 0.2327, 0.0375, 0.0031, 0.0001}</td>
</tr>
</tbody>
</table>

**Table 2.** Invariants corresponding to SH’s with $l = 2$.

<table>
<thead>
<tr>
<th>$l = 2$</th>
<th>$(I_1, \ldots, I_6)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_2^{-2}$</td>
<td>(0, -0.3480, 0.0104, 0, 0)</td>
</tr>
<tr>
<td>$Y_2^{-1}$</td>
<td>(0, -0.3480, 0.0104, 0, 0)</td>
</tr>
<tr>
<td>$Y_2^0$</td>
<td>(0.0002, -0.3480, 0.0545, 0.0104, -0.0011, -0.0001)</td>
</tr>
<tr>
<td>$Y_2^1$</td>
<td>(0, -0.3480, 0.0104, 0, 0)</td>
</tr>
<tr>
<td>$Y_2^2$</td>
<td>(0, -0.3480, 0.0104, 0, 0)</td>
</tr>
</tbody>
</table>
Table 3. Invariants corresponding to SH’s with \( l = 4 \).

<table>
<thead>
<tr>
<th>( l = 4 )</th>
<th>((\lambda_1, \ldots, \lambda_6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \hat{Y}_{-3} )</td>
<td>((0, -1.5665, 0, 0, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{-2} )</td>
<td>((0, -1.5665, 0, 0.6010, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{-1} )</td>
<td>((0, -1.5665, 0, 0.1628, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{0} )</td>
<td>((0.003, -1.5665, 0.2837, 0.3205, 0.0407, 4 \times 10^{-6}))</td>
</tr>
<tr>
<td>( \hat{Y}_{1} )</td>
<td>((0, -1.5665, 0, 0.1628, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{2} )</td>
<td>((0, -1.5665, 0, 0.6010, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{3} )</td>
<td>((0, -1.5665, 0, 0.6134, 0, 0))</td>
</tr>
<tr>
<td>( \hat{Y}_{4} )</td>
<td>((0, -1.5665, 0, 0, 0, 0))</td>
</tr>
</tbody>
</table>

3.2 Phantom data

We consider an existing phantom containing crossing fibers at an angle of 90° and corresponding diffusion MRI data acquired in 200 directions at a b-value of 2000 [20]. We compute the fourth-order orientation distribution functions from the HARDI signal and the eigenvalues and principal invariants of the corresponding tensors [7]. The latter are given in Figure 2.

Fig. 2. Principal invariants on a 90° fiber crossing phantom. Top row: \( \lambda_1, \lambda_2, \lambda_3 \). Bottom row: \( \lambda_4, \lambda_5, \lambda_6 \).
It can be seen from the figure that $I_1$ shows a considerable amount of noise, which is much less apparent for the rest of the invariants. The resulting invariants show some contrast between the crossing and isotropic background, and between the crossing and single fiber regions. The latter is the case for $I_4$ to $I_6$. Based on the results of the previous section, we expect $I_4$ to be larger in areas where tensors have a high $l = 4$ SH contribution (such as crossings), and lower where such components are small with respect to the $l = 2$ ones (single fibers). This is indeed reflected by $I_4$ in Figure 2. However, similar results can be seen for $I_5$ and $I_6$. In this case we cannot extrapolate conclusions from the SH invariants since they are both zero for most of them.

On the other hand, one would expect more coherence for each invariant map within homogeneous phantom regions (vertical single fiber, horizontal single fiber and crossing region). Invariants in these areas are indeed similar but the range of invariant values between different regions is rather broad. More advanced visualization techniques may help improving this aspect.

### 3.3 Real brain data

We perform experiments on real brain diffusion MRI data, consisting of ten horizontal slices positioned through the corpus callosum and centrum semiovale [21]. The data were acquired with 132 gradient directions at a $b$-value of 1000 s/mm$^2$ and a voxel size of 2.0 × 2.0 × 2.0 mm. Results of the computed invariants are shown in Figure 3 (middle slice). The scalar maps $I_3$ to $I_6$ (middle and bottom row) show high variability. It is further not straightforward to derive immediate information from the results.

### 4 Discussion and Outlook

In this paper we present the novel idea of considering fourth-order tensor invariants as building blocks for scalar measures in HARDI. The purpose of such measures is to extract relevant information on organization and anisotropy properties of white matter fibers by reducing the complex data to meaningful scalars. A number of HARDI measures have been proposed in the literature but none of them are based on higher-order tensor invariants. This is somewhat surprising since the most popular measure in DTI, fractional anisotropy, is an invariant of the second-order diffusion tensor.

We show that invariants on spherical harmonic tensors have a number of interesting features. However, these are not immediately seen on real phantom HARDI data. The phantom invariants show some sensitivity at fiber crossings with respect to the isotropic background and single fiber areas but quantifying this is hard. Invariant maps of real brain data are not immediately informative at this stage. It would be interesting to relate the principal invariants to GA and SE. These are rotationally invariant measures and can therefore be expressed in
Fig. 3. Principal invariants on real brain data. Middle slice is shown. Top row: $I_1, I_2$. Middle row: $I_3, I_4$. Bottom row: $I_5, I_6$.

terms of the proposed higher-order invariants. A comparison between results of individual invariants and those given by GA or SE is for this reason not representative.

The proposed invariants can be used to define new scalar measures in HARDI which will immediately be rotationally invariant. On the other hand, the invariants feature space can be used for voxel classification purposes as it is done in [22] for fourth-order SH coefficients, with the advantage of a reduced number of parameters (from 15 to only 6). Future work will include the computation of the principal invariants on simulated tensor crossings, as an intermediate step between spherical harmonic tensors and phantom HARDI data, and new experiments on real brain HARDI data. In this way we can gain more insight in the interpretation of invariants, allowing for the construction of well-motivated HARDI measures. In addition, invariants of tensors of order higher than four will be considered.
We present preliminary results on fourth-order tensor invariants of real phantom and brain HARDI data. Further work is required to investigate which information can potentially be derived from invariant-related maps. We conclude that higher-order tensor invariants are a valuable but yet unexplored tool which are worth further research in the context of HARDI scalar measures.

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References

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