Orthogonal Tensor Invariants and the Analysis of Diffusion Tensor Magnetic Resonance Images

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This paper outlines the mathematical development and application of two analytically orthogonal tensor invariants sets. Diffusion tensors can be mathematically decomposed into shape and orientation information, determined by the eigenvalues and eigenvectors, respectively. The developments herein orthogonalize the tensor shape using a set of three orthogonal invariants that characterize the magnitude of isotropy, the magnitude of anisotropy, and the mode of anisotropy. The mode of anisotropy is useful for resolving whether a region of anisotropy is linear anisotropic, orthotropic, or planar anisotropic. Both tensor trace and fractional anisotropy are members of an orthogonal invariant set, but they do not belong to the same set. It is proven that tensor trace and fractional anisotropy are not mutually orthogonal measures of the diffusive process. The results are applied to the analysis and visualization of diffusion tensor magnetic resonance images of the brain in a healthy volunteer. The theoretical developments provide a method for generating scalar maps of the diffusion tensor data, including novel fractional anisotropy maps that are color encoded for the mode of anisotropy and directionally encoded colormaps of only linearly anisotropic structures, rather than high fractional anisotropy structures. Magn Reson Med 55: 136–146, 2006. © 2005 Wiley-Liss, Inc.

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The utility of magnetic resonance imaging (MRI) to characterize biologic tissue is amplified by analysis and visualization methods that help researchers to see and understand the structures within the data. Tensor-valued imaging is an increasingly important source of information about tissue structure and dynamics, such as with diffusion tensor MRI (DT-MRI), and strain tensors derived from displacement encoded MRI. An effective and established way of describing structure in tensor fields is through a function that maps tensors to more readily understood scalar metrics. The medical imaging literature provides a variety of such metrics (e.g., bulk mean diffusivity, fractional anisotropy).

This paper uses a combination of mathematics and visualizations to generate a rigorous and intuitive exposition of tensor shape, characterized by sets of orthogonal tensor invariants. Each invariant set decomposes tensor shape with an orthogonal basis. When invariants have application-specific significance (as they do in DT-MRI imaging), orthogonality is a useful property of an invariant set, because it isolates the measurement of variation in one physiologic property from variations in another. These sets of orthogonal tensor invariants are then used to create informative visualizations of tensor field structure. The result is the establishment of two sets of orthogonal tensor invariants that incorporate the established use of fractional anisotropy (FA) and apparent diffusion coefficient (ADC).

Diffusion tensors are symmetric and thus can be decomposed into an eigensystem of three real eigenvalues and three mutually orthogonal eigenvectors. We adopt the terminology that tensor “shape” refers to those degrees of freedom in tensor values (components of the matrix representation of a tensor) spanned by changes in the eigenvalues, while keeping eigenvectors fixed. “Orientation,” on the other hand, refers to the complementary degrees of freedom associated with changes in the eigenvectors, while keeping the eigenvalues fixed. Defining shape and orientation in terms of the tensor eigensystem coincides with the standard visualization of the tensor as an ellipsoid, with its orientation determined by aligning its axes with the eigenvectors and scaling its axes by the eigenvalues. Note that when visualizing diffusion tensors as an ellipsoidal diffusion probability profile, the square root of the eigenvalues is typically used.

The methods presented here will be formally described in terms of tensor invariants. Invariants are the preferred scalar metric because they are independent of the coordinate system of the tensor’s matrix representation and thus represent intrinsic measures of the tensor. We use “shape metric” to refer to any scalar invariant that quantifies some salient geometric property of tensor shape, such as overall size or eccentricity (anisotropy). Although we primarily adopt the terminology and metrics of the DT-MRI literature and demonstrate results on DT-MRI data, the mathematical framework described applies to any second-order symmetric tensor field, such as strain tensor images.

The established analysis of DT-MRI data relies on scalar invariants of tensors as a result of the empiric observation that tensor shape is an indicator of the underlying tissue microstructure and organization. One class of tensor invariants is used to quantify some aspect of overall diffusion tensor magnitude, including tensor norm and tensor trace. The tensor trace is proportional to the ADC (also termed the bulk mean diffusivity). Although the ADC can be measured without a full tensor acquisition, the quantity is exactly one third the tensor trace, or the mean of the tensor eigenvalues. The ADC has been widely reported as an effective indicator for acute ischemic stroke (1). Another class of tensor invariants includes the various anisotropy measures that quantify the extent to which the diffusion rate is direc-
tionally dependent, or the magnitude of anisotropy. Many anisotropy indices popular in DT-MRI (FA, RA, volume ratio, $c_2$) (2,3) are invariant and are therefore shape metrics. Fractional anisotropy is used in studies of chronic and acute cerebral ischemia, multiple sclerosis, metabolic disorders, epilepsy, and brain tumors (4).

As noted by others, however, tensor shape is intrinsically a trivariate quantity (5). No two scalar measures (e.g., tensor norm and FA) can account for the degrees of freedom represented by the three eigenvalues. In order to describe the third degree of freedom we adopt the term “tensor mode” from Criscione et al. (6) to refer to a shape metric that quantifies the type of tensor anisotropy, as it ranges from linear anisotropy, to orthotropy, to planar anisotropy. Tensor mode has not been described in the DT-MRI literature even though it orthogonally complements common tensor magnitude and anisotropy measures. In particular, tensor mode may be useful for quantifying uncertainty in fiber orientation (principal eigenvector), a topic examined by Jones (7).

The distinction between linear and planar anisotropy (measured by tensor mode) is significant in two related contexts. First, previous analysis of partial voluming in DT-MRI demonstrated a bias toward planar anisotropy caused by blending of adjacent regions of linear anisotropy along orthogonal orientations (6). Such white matter fibers configurations include the right–left transpontine tracts ventral to the inferior–superior corticospinal tracts in the brainstem and the right–left tracts of the corpus callosum inferior to the anterior–posterior cingulum bundles. Planar anisotropy can also arise in more complex configurations, rather than mere adjacency of orthogonal fiber orientations. Previous work in visualizing regions of significant planar anisotropy characterized locations where populations of differently oriented fibers apparently mix at a fine scale, far below that of the image resolution (9). Locations with this configuration include the medial–lateral fanning of the predominant anterior–posterior direction of the superior longitudinal fascicle and the intersection of the medial–lateral tracts of the corpus callosum with the inferior–superior tracts of the corona radiata. More generally, Tuch et al. demonstrated that in the brain, the residual error of fitting a tensor model to high-angular resolution DWI increases with planarity of the tensor (10). Because tensor mode encapsulates the distinction between linear and planar anisotropy, it is appropriate to isolate this variable for the purposes of analyzing and processing diffusion tensor images.

Previous work has recognized the importance of orthogonal tensor invariant measures. The work of Bahn (5) outlined various invariant measures, but the mathematics were not in terms of familiar tensor functions. The work of Criscione et al. (6) demonstrated the mathematics defining a set of mutually orthogonal tensor invariants, but was not applied to DT-MRI, nor did it show that an invariant set containing fractional anisotropy exists. The principal invariants that arise naturally from the tensor’s characteristic equation ($l_1$, $l_2$, and $l_3$) are not mutually orthogonal (derivation not shown), nor are the invariant measures of linear, planar, and spherical tensor components of Westin et al. (3). Lastly, fractional anisotropy and tensor trace have become a common invariant pair used in the analysis of DT-MRI data, but these measures are not orthogonal (see Appendix B). However, tensor trace and fractional anisotropy are each an essential member of an orthogonal tensor invariant set.

Throughout this paper, we use visualizations to demonstrate the theoretical developments and to improve the interpretability of DT-MRI data. Visualizing the space of tensor shape itself illustrates properties of invariant sets, irrespective of any particular data. We also introduce two- and three-dimensional colormaps of tensor shape, in which tensor size, anisotropy, and mode are mapped to color brightness, saturation, and hue. This results in improved fractional anisotropy maps and improved directionally encoded colormaps.

**THEORY**

Invariants are scalar-valued functions of a tensor variable that are independent of the choice of coordinate system. In order to determine whether two invariants are mutually orthogonal one must first calculate the gradient of the invariant function. The gradient of a scalar-valued function of a tensor variable is itself a tensor, much as the gradient of a scalar-valued function of a vector is itself a vector. Two elements (vectors or tensors) are orthogonal if and only if their inner product is zero. For tensors the inner product operator is termed contraction and is denoted by a colon (:). If two tensors $U$ and $V$ are orthogonal this implies that

$$U:V = \text{tr}(UV^T) = 0. \quad [1]$$

Therein, tr() is the trace operator and superscript T indicates transposition. A mutually orthogonal set of three tensors $U$, $V$, and $W$ therefore consists of three tensors for which the following is true: $U:V = 0$, $V:W = 0$, and $W:U = 0$.

The tensor magnitude is defined using tensorial contraction and is equivalent to the Frobenius norm of the tensor’s matrix representation.

$$\text{norm}(A) = \sqrt{A:A} \quad [2]$$

Appendix A outlines additional properties of tensorial contraction. The mechanics of computing invariant gradients and of proving the orthogonality between invariant gradients is also outlined in Appendix A. The expressions throughout use standard analysis functions (trace, determinant, and norm), but are shown equivalently expressed in terms of individual eigenvalues ($\lambda_1$, $\lambda_2$, $\lambda_3$) and the first three central moments of the eigenvalues $\mu_1$ (mean), $\mu_2$ (variance), and $\mu_3$.

In order to enumerate distinct sets of orthogonal tensor invariants we categorize sets based on the number of dimensionless invariants and draw an analogy to the three most basic coordinate systems for three-dimensional space: Cartesian, cylindrical, and spherical. A set of three dimensionless measures is not considered as it cannot quantify overall tensor size and therefore cannot capture all degrees of freedom in tensor shape. A Cartesian set of three mutually orthogonal dimensionful tensor invariants is formed by the eigenvalues themselves; however, they
are not considered because fundamental attributes of tensor shape (e.g., size, anisotropy) are not isolated.

Cylindrical Invariant Set

An orthogonal tensor invariant set consisting of a single dimensionless invariant forms a basis for tensor shape decomposition that is analogous to a cylindrical coordinate system; both are defined by two dimensionful parameters and one dimensionless parameter.

In order to define the cylindrical set of orthogonal tensor invariants it is convenient to decompose a tensor $\mathbf{A}$ as follows,

$$
\mathbf{A} = \tilde{\mathbf{A}} + \hat{\mathbf{A}},
$$

where $\tilde{\mathbf{A}}$ represents the isotropic part of the tensor and $\hat{\mathbf{A}}$ represents the anisotropic (deviatoric) part of the tensor where each part is defined as follows,

$$
\tilde{\mathbf{A}} = \frac{1}{3} \text{tr}(\mathbf{A}) \mathbf{I} = \frac{1}{3} (\mathbf{A} : \mathbf{I} \mathbf{I}),
$$

$$
\hat{\mathbf{A}} = \mathbf{A} - \frac{1}{3} \text{tr}(\mathbf{A}) \mathbf{I} = \mathbf{A} - \frac{1}{3} (\mathbf{A} : \mathbf{I} \mathbf{I}).
$$

This decomposition was the basis for the development of a set of orthogonal tensor invariants with only one dimensionless member first introduced by Criscione et al. for the development of hyperelastic strain energy functions with orthogonal response terms (6). Criscione et al. describe the following set of invariants:

$$
K_1 = \text{tr}(\tilde{\mathbf{A}}) \tag{6}
$$

$$
K_2 = \text{norm}(\tilde{\mathbf{A}}) \tag{7}
$$

$$
K_3 = \text{mode}(\hat{\mathbf{A}}) \tag{8}
$$

Note that Eqs. [7] and [8] specifically operate on the anisotropic part of $\mathbf{A}$. In Eq. [8] the mode operator is defined by

$$
\text{mode}(\hat{\mathbf{A}}) = 3 \sqrt[3]{6} \text{det}(\hat{\mathbf{A}}/\text{norm}(\hat{\mathbf{A}})). \tag{9}
$$

The determinant operator is det().

This set of invariants orthogonally decomposes the tensor into three intuitively meaningful components where $K_1$ represents the magnitude of isotropy (i.e., mean diffusivity in the case of diffusion), $K_2$ represents the magnitude of anisotropy, and $K_3$ represents the mode of anisotropy. By analogy to a polar cylindrical coordinate system $K_1$ is the longitudinal component, $K_2$ is the radial component, and $K_3$ is the azimuthal coordinate. For symmetric, positive-definite tensors $K_1$ and $K_2$ are both defined on the interval $[0, +\infty)$. $K_3$ is defined on the interval $[-1, +1]$ where $K_3 = -1$ indicates a planar anisotropic tensor (two large diffusion tensor eigenvalues and one small eigenvalue), $K_3 = 0$ indicates an orthotropic tensor, and $K_3 = 1$ indicates a linear anisotropic tensor (one large diffusion tensor eigenvalue and two small eigenvalues). Orthotropic tensors indicate a diffusive state in between linear and planar anisotropy wherein the three eigenvalues are distinct. For completeness we note that an isotropic tensor has three equal eigenvalues. The mutual orthogonality of the $K_i$ invariant set is outlined in Appendix B.

Using Eqs. [6] and [7] the tensor $\mathbf{A}$ can then be expressed as

$$
\mathbf{A} = \frac{1}{2} K_1 \mathbf{I} + K_3 \mathbf{\Phi}, \tag{10}
$$

where

$$
\mathbf{\Phi} = \tilde{\mathbf{A}}/\text{norm}(\tilde{\mathbf{A}}) \tag{11}
$$

is a tensor specifying how the anisotropy contributes to the tensor $\mathbf{A}$. Note that the determinant of $\Phi$ is proportional to the tensor mode.

For the purpose of computation it is sometimes useful to use different parameterizations of the same invariants. It can be shown that $K_1 = \text{tr}(\mathbf{A}) = \lambda_1 + \lambda_2 + \lambda_3 = 3 \mu_1, K_2 = \text{norm}(\tilde{\mathbf{A}}) = \sqrt{(\lambda_1 - \mu_1)^2 + (\lambda_2 - \mu_1)^2 + (\lambda_3 - \mu_1)^2} = \sqrt{3 \mu_2}$, and $K_3 = \text{mode}(\hat{\mathbf{A}}) = \lambda_1 \lambda_2 \lambda_3/\text{norm}(\hat{\mathbf{A}})^3 = \sqrt{2\mu_3 \mu_2^{-3/2}}$. Therefore, these measures can be calculated with or without eigensystem decomposition. The later definition for $K_3$ demonstrates that $K_3$ is proportional to the skewness of the eigenvalues ($\mu_3 \mu_2^{-3/2}$).

Spherical Invariant Set

An orthogonal tensor invariant set consisting of two dimensionless invariants forms a basis for tensor shape decomposition that is analogous to a spherical coordinate system in that they both employ two dimensionless parameters and one dimensionful parameter. A mutually orthogonal invariant set containing fractional anisotropy as a member is defined as follows:

$$
R_1 = \text{norm}(\mathbf{A}) = \sqrt{\tilde{\mathbf{A}} : \tilde{\mathbf{A}}} \tag{12}
$$

$$
R_2 = \text{FA}(\mathbf{A}) = \sqrt[3]{3 \text{ norm}(\tilde{\mathbf{A}}) \text{ norm}(\hat{\mathbf{A}})} \tag{13}
$$

$$
R_3 = K_3 = \text{mode}(\hat{\mathbf{A}}). \tag{14}
$$

For symmetric, positive-definite tensors $R_1$ is defined on the interval $[0, +\infty), R_2$ is defined on $[0, 1]$, and $R_3$ is defined on $[-1, +1]$. The mutual orthogonality of the $R_i$ invariant set is proven in Appendix B. $R_1$ is a measure of tensor magnitude, $R_2$ is the fractional anisotropy, and $R_3$ is a measure of the mode of anisotropy and is equivalent to $K_3$ (Eq. [8]). Part of the utility of the $R_i$ invariant set is that it contains a measure of anisotropy (FA) that is commonly used in the analysis of DT-MRI. Calculation of the invariants in Eqs. [12–14] does not require the calculation of eigenvalues, but we note that $R_1 = \text{norm}(\mathbf{A}) = \sqrt{\lambda_1^2 + \lambda_2^2 + \lambda_3^2} = \sqrt{3 \mu_1^2 + 3 \mu_2}, R_2 = \text{FA}(\mathbf{A}) = \sqrt[3]{3 \mu_3 \mu_2^{3/2} + (\lambda_2 - \mu_1)^2 + (\lambda_3 - \mu_1)^2}/R_1 = \sqrt{3 \mu_2 + 3 \mu_2^{3/2}}$, and $R_3 = K_3 = \text{mode}(\hat{\mathbf{A}}) = \lambda_1 \lambda_2 \lambda_3/\text{norm}(\hat{\mathbf{A}})^3 = \sqrt{2\mu_3 \mu_2^{-3/2}}$.

Beside including a widely used measure of anisotropy (FA), we submit that this tensor invariant set contains a suitable surrogate for mean diffusivity (norm($\mathbf{A}$)), as well
as containing a useful measure of the kind of tensor anisotropy (mode(\(A_\tilde{\theta}\))).

Utility of Tensor Invariants Sets

The one and two dimensionless invariant sets are natural, because they contain overall size as a fundamental aspect of shape (either trace or norm). Furthermore, each set contains a measure of the magnitude of anisotropy and both sets share a measure of the kind of anisotropy as characterized by the mode of the tensor. As an example of the utility of this orthogonal invariant set, note that the empiric constancy of mean diffusivity (\(K_1\)) in the parenchyma (11) means that tensor shape variations associated with anatomic structural variation must lie along the other two axes of tensor shape, namely the magnitude of anisotropy (\(K_2\)) and the mode of anisotropy (\(K_3\)).

METHODS

Essential to the analysis of diffusion tensor fields is visualization of the underlying data. This can take the form of scalar, vector, or tensor field maps that are encoded by color, intensity, opacity, shape functions (glyphs), and a variety of combinations of the same. Common visualization schemes include tensor invariant scalar maps, directionally encoded colormaps (12), and three-dimensional glyph renderings (13).

Visualizing the Space of Tensor Invariants

The space of tensor shape (invariants) can be visualized by volume renderings of invariant isosurfaces over the space of diagonal tensors. Figure 1 displays isosurfaces of each of the three invariants contained within each of the two orthogonal tensor invariant sets. Each surface represents the range of eigenvalue triplets that span a constant invariant value.

Visualizing Space of FA and Mode

In the analysis of diffusion tensor data it is essential to appreciate that fractional anisotropy alone is not sufficient to characterize the anisotropy of the diffusion tensor. The mode of anisotropy is an important orthogonal descriptor. Specifically, it is inappropriate to associate high fractional anisotropy with organized linear anisotropy or fibrous structures and tensor mode can be used to distinguish high linear anisotropy from high planar anisotropy. Figure 2 demonstrates superquadric glyph (13) renderings of tensors with constant norm. Using the orthogonal decomposition of norm(\(A\)), FA(\(A\)) and mode(\(\tilde{A}\)) outlined under Theory, the tensor invariant space can be mapped visually using superquadric glyphs (Fig. 2). Glyphs that lie along arcs at a fixed distance from the isotropic tensor (FA = \(1/\sqrt{2}\), mode is indeterminate) have equal fractional anisotropy, but a range of mode. For values of FA up to \(1/\sqrt{2}\) the planar-anisotropic and linear-anisotropic cases are not distinguishable based upon FA alone, but become distinguishable when mode is calculated.

Visualization of Tensor Invariant Maps

The orthogonal tensor invariant sets outlined under Theory can be used to display information about the diffusion tensor data in a compact form. For the display of norm(\(A\)), FA(\(A\)), trace(\(A\)), norm(\(\tilde{A}\)), and mode(\(\tilde{A}\)), it is sufficient to generate scalar grayscale images that reflect the underlying invariant measure within each image pixel (Fig. 3).

Visualization of Tensor Orientation and Mode

Directionally encoded colormaps provide a means for displaying the orientation of anisotropic structures. To accomplish this, the primary eigenvector components are encoded into the red, green, and blue channels of a color image. The highly anisotropic data are then accentuated by saturating the color intensity by some measure of anisotropy (typically fractional anisotropy) (12). Figure 4 dem-
FIG. 2. Demonstration of the space of anisotropy decomposed into two orthogonal channels: fractional anisotropy \((FA = R_3)\) and mode \((= R_3 = K_3)\). Each glyph represents the shape of diffusion tensors with constant tensor norm rendered with superquadric glyphs. Increasing distance from the top left spherical glyph indicates increasing \(FA\), whereas the angular deviation from the left edge indicates increasing mode as it transitions from planar anisotropic \((mode = -1)\), to orthogonal \((mode = 0)\), to linear anisotropic \((mode = 1)\). Glyphs along constant radii \((constrained to an arc)\) are of constant fractional anisotropy, but of varying mode. This figure explicitly demonstrates that increases in \(FA\) do not necessarily indicate increasing linear anisotropy. The space of \(FA\) and mode is correctly diagrammed as an isosceles triangle; note that isocontours of \(FA\) are orthogonal to isocontours of mode.

Demonstrates a fractional anisotropy map color encoded for the tensor mode. The hue is determined by a “rainbow” color map of the tensor mode, while the value (brightness) is modulated by fractional anisotropy, and saturation is fixed. Saturated blues indicate linear anisotropy and saturated reds indicate planar anisotropy. If the underlying tensor is planar anisotropic then the orientation of the primary eigenvector is indeterminate within a plane of rotation. Thus, the generation of maps that highlight eigenvectors only of highly linear structures are different than those that highlight eigenvectors in regions of high fractional anisotropy. To that end, Fig. 5 contrasts directionally encoded color maps of the primary eigenvector \((12)\), which do and do not assign saturated colors to regions of planar anisotropy \((high tensor mode)\).

Estimates of mode are expected to be highly variable for low anisotropy, as noise will increasingly dominate the measure. The importance of tensor mode increases as fractional anisotropy increases. The display of mode data is therefore improved by modulating the color saturation by the fractional anisotropy. This provides a way to map orthogonal tensor shape attributes to orthogonal color attributes. Such maps \((Figs. 4 \& 5)\) indicate regions of combined high fractional anisotropy and low mode \((planar anisotropy)\) wherein fiber tracking might be problematic. Lastly, in Fig. 6 we demonstrate the color mapping of the complete orthogonal invariant set of norm(\(A\)), \(FA(\bar{A})\), mode(\(\bar{A}\)) and \(\text{tr}(\bar{A})\), norm(\(\bar{A}\)), mode(\(\bar{A}\)) to the orthogonal color components brightness, saturation, and hue.

DT-MRI Data Acquisition

Diffusion tensor magnetic resonance images were acquired in a single healthy volunteer after obtaining a signed statement of informed consent. All imaging procedures followed the institution’s guidelines for patient safety.

Diffusion tensor magnetic resonance images were acquired using the manufacturer’s diffusion weighted twice-refocused spin (dual spin) echo EPI pulse sequence with 31 gradient directions. The image parameters on the 3.0-T Signa VH MR scanner (General Electric, Waukesha, WI, USA) were as follows: field of view, 24 cm; slice thickness, 3.5 mm; imaging matrix, 128 × 128; repetition time, 1150 ms; echo time, 86.9 ms; bandwidth, ±62.5 kHz; number of interleaved slices, 32; and \(b\)-value = 750 s/mm\(^2\). The images were postprocessed to correct for eddy-current effects. The components of the diffusion tensor were solved using linear regression.

RESULTS

Figure 1 graphically demonstrates the results of the analytic proofs provided in Appendix B by rendering isosurfaces of each member of each tensor invariant set. It is apparent in Fig. 1 that the isosurfaces of each invariant set form mutually orthogonal surfaces. It is also apparent that the isosurfaces of tensor trace are not orthogonal to the isosurfaces of fractional anisotropy. This fact is mathematically derived at the end of Appendix B. Fractional anisotropy is necessarily an incomplete description of tensor anisotropy. Figure 2 demonstrates the ambiguity associated with only considering the magnitude of anisotropy, specifically \(FA\). For fractional anisotropy measures less than 1/√\(2\) the full range of tensor modes is possible. Tensor mode orthogonally complements fractional anisotropy and helps resolve the potential ambiguity associated with calculating fractional anisotropy alone.

Figure 3 demonstrates scalar maps of each of the tensor invariants from the two proposed sets of orthogonal tensor invariants. Regions of the image outside of the patient have been masked to improve the readability of the maps. The previously observed empiric constancy of the tensor trace \((11)\) is evident throughout the parenchyma in Fig. 1a. Similar contrast is evident in the scalar map of tensor norm \((Fig. 1d)\), indicating that if fractional anisotropy is the preferred measure of the magnitude of anisotropy then tensor norm is a suitable surrogate for tensor trace and is also orthogonal to fractional anisotropy. The maps of norm(\(\bar{A}\)) and \(FA\) also indicate similar contrast largely because \(FA\) is simply norm(\(\bar{A}\)) normalized by norm(\(A\)), which is also relatively constant within the parenchyma. Measures of mode(\(\bar{A}\)) indicate mostly linear anisotropy in the corpus callosum, internal capsule, and cingulum and are more variable in areas of low fractional anisotropy where the measure may be governed more by noise than anisotropy of the diffusion process. Note the dark band of low tensor mode between the corpus callosum and the posterior cingulum bundles, indicating a region of planar anisotropy \((low tensor mode)\). The same slice is used in Figs. 3–6 and anatomic labels are included in Fig. 4.
edge indicates that blue hues represent linear anisotropy, green hues represent orthotropy, and red hues represent planar anisotropy. The intensity is modulated by fractional anisotropy. Note that in addition to highly fractional anisotropic regions of linear anisotropy (i.e., corpus callosum, blue regions), large areas of high fractional anisotropy indicate planar (red regions) and orthotropic (green regions) anisotropy. Note also the transition from linear-orthotropic-planar-orthotropic-linear anisotropy as the primary fiber direction changes from predominantly in the left–right direction within the splenium of the corpus callosum to anterior–posterior in the cingulum. Furthermore, linear anisotropic regions are generally separated from planar anisotropic regions by regions of orthotropic anisotropy throughout areas of high fractional anisotropy. Such tensor mode transitions likely arise from the partial volume effects of imaging two nonparallel fiber structures within a single voxel.

Figure 5 demonstrates both a directionally encoded colormap of the primary eigenvector with color brightness modulated by the fractional anisotropy (Fig. 5a) and a directionally encoded colormap of the primary eigenvector that is intensity modulated by a product of fractional anisotropy and tensor mode (Fig. 5b). The advantage of the latter map is that it only indicates a primary eigenvector direction when that direction is well-defined. In areas of planar anisotropy, where the direction of the primary eigenvector is indeterminate within a plane of rotation rendering a single eigenvector direction is not meaningful. Note in Fig. 5b that most anatomic structures appear decreased in their extent when compared to Fig. 5a. Notable exceptions include the corpus callosum and the cingulum. A band of low tensor mode is visible in the boundary between the corpus callosum and the cingulum indicating planar anisotropy. This probably arises within voxels that contain corpus callosum fibers oriented in the right–left direction and cingulum fibers oriented in the anterior–posterior direction.

Figure 6 demonstrates complete mappings of the two orthogonal tensor invariants sets to the hue, saturation, and value channels of a color image. Figure 6a maps the hue, saturation, and value to mode($\hat{\mathbf{A}}$), FA($\mathbf{A}$), and norm($\mathbf{A}$) and Fig. 6b maps the hue, saturation, and value to mode($\hat{\mathbf{A}}$), norm($\hat{\mathbf{A}}$), tr($\mathbf{A}$). Both maps indicate high magnitude of anisotropy with high color saturation and the hue indicates the mode of anisotropy (blue, linear anisotropic; green, orthotropic; red, planar anisotropic). The magnitude of isotropy is indicated by the color value and is apparent as a grayscale map of the brain in areas of low magnitude of anisotropy. The hue-saturation-value maps of the $K_i$ invariants have more saturated colors because the
measure of the magnitude of anisotropy is not normalized by the magnitude of the isotropic component of the tensor as is the case with the $R_i$ invariants use of fractional anisotropy. This increases the color saturation in areas of high magnitude of anisotropy, but also in areas of low magnitude of anisotropy as is apparent in the right lateral ventricular space adjacent to the corpus callosum.

**DISCUSSION**

The formulation of two possible orthogonal invariant sets provide novel bases for the analysis and decomposition of diffusion tensor data that eliminate the mathematical dependence between the invariants within the set. Aside from the invariants that arise from the solution to the tensor’s characteristic equation, tensor invariants have not been considered as sets. In previous studies when various invariants, typically tensor trace and fractional anisotropy, were combined in an overall analysis the chosen metrics were not orthogonal. Furthermore, previous studies analyzed the correlation of tensor trace and fractional anisotropy (14). While there can be physiologic correlation between these two measures we have shown that there is, in fact, mathematical correlation as well. To that end it is judicious to analyze the correlation of orthogonal tensor invariants in future studies.

It is common to saturate the colors in a directionally encoded colormap using the fractional anisotropy map. It is perhaps more judicious to saturate the colormap based on some measure of the confidence in the directionality of the primary eigenvector in addition to the magnitude of anisotropy. To that end, maps that saturate colors based on fractional anisotropy and tensor mode can be generated to highlight regions of linear anisotropy (Fig. 5b).

Fiber tracking algorithms will likely benefit from the use of orthogonal tensor invariant sets. Fiber tracking algorithms attempt to define large-scale connectivity within the brain, but the tracking is compounded by noise, crossing fibers, and primary eigenvector confidence measures. Fractional anisotropy is a poor surrogate for a measure of

**FIG. 4.** Hue-saturation-value map of tensor mode and fractional anisotropy. The tensor mode modulates the hue while fractional anisotropy modulates the value. The saturation is constant and equal to 1. The shape-color legend indicates the mode of anisotropy. Blue structures are indicative of linear anisotropy, green of orthotropy, and red of planar anisotropy. The corpus callosum and the cingulum are observed to be a largely linear anisotropic structures, but other structures with high fractional anisotropy are a mix of linear, orthotropic, and planar anisotropy. Note the transition from linear-orthotropic-planar-orthotropic-linear anisotropy in between the corpus callosum and the cingulum.

**FIG. 5.** Directionally encoded colormaps of the primary eigenvectors. (a) demonstrates the magnitude of the primary eigenvector components encoded into the red, blue, and green channels and intensity modulated by fractional anisotropy. (b) demonstrates the magnitude of the primary eigenvector components encoded into the red, blue, and green channels and intensity modulated by fractional anisotropy and the tensor mode. (b) highlights the orientation only of structures with high linear anisotropy for which the primary eigenvector is well determined. High-intensity structures indicate high linear anisotropy. Low-intensity structures indicate low fractional anisotropy or planar anisotropy and ambiguous primary eigenvector directions. Note the intensity difference along the border of the corpus callosum and the cingulum.
APPENDIX A

Tensorial Contraction

This Appendix introduces the basic tensor mathematics needed to define the gradient of a tensor function. Recall the definition of tensorial contraction (tensorial inner product) connoted by a colon (:) as

$$A:B = \text{tr}(AB^T) = \text{tr}(A^T B) = \text{tr}(BA^T) = \text{tr}(B^T A),$$  \[A1\]

where \(\text{tr}()\) is the trace operator and superscript \(T\) denotes transposition. Tensorial contraction is both distributive and commutative,

$$A:(B + C) = A:B + A:C, \hspace{1cm} [A2]$$

$$A:B = B:A. \hspace{1cm} [A3]$$

Other useful properties of tensorial contraction follow:

$$A:\alpha B = \alpha (A:B), \hspace{1cm} [A4]$$

$$A:I = \text{tr}(A), \hspace{1cm} [A5]$$

$$A:(BC) = (B^T A):C = (AC^T):B. \hspace{1cm} [A6]$$

Gradients of Invariant Functions

A tensor invariant \(\Psi\) is a scalar-valued function of a tensor argument, \(\Psi(A) = s\). The gradient of \(\Psi\), \(\partial \Psi / \partial A\), can be defined in terms of the Taylor expansion of \(\Psi(A + dA)\):

$$\Psi(A + dA) = \Psi(A) + \frac{\partial \Psi}{\partial A} : dA + O(dA^2) = \Psi(A) + \frac{\partial \Psi}{\partial A} : dA. \hspace{1cm} [A7]$$

Note that \(O(dA^2) = 0\) because second-order terms approach zero faster than does infinitesimal \(dA\). In the following discussion, the increment in the tensor \(A\) is \(dA\), and the increment of \(\Psi\) is

$$d\Psi = \Psi(A + dA) - \Psi(A) = \frac{\partial \Psi}{\partial A} : dA. \hspace{1cm} [A8]$$

Equation \([A8]\) demonstrates that for infinitesimal \(dA\) the gradient of a tensor invariant represents the linear mapping from one incremental space \((dA)\) to another \((d\Psi)\).
The procedure for defining $\partial \Psi / \partial \mathbf{A}$ for various scalar valued tensor functions is to take the variation of the function $\Psi(\mathbf{A})$ and manipulate it until it is in the form of Eq. [A8]. It is often helpful to use the distributive or commutative properties of tensorial contraction (Eqs. [A2] and [A3]), use Eq. [A4] for rearranging constant coefficients, or replace or linearize expressions so that they are a function of $\mathbf{tr}(\mathbf{A})$ and substitute this for (A3) using Eq. [A5], or to rearrange complex terms containing $\partial \mathbf{A}$ using Eq. [A6]. Once the gradient functions for each invariant within a set $(\Psi_i(\mathbf{A}), i = 1, 2, 3)$ are defined we need only prove that

$$\frac{\partial \Psi_i(\mathbf{A})}{\partial \mathbf{A}} \cdot \frac{\partial \Psi_j(\mathbf{A})}{\partial \mathbf{A}} = 0, \quad i \neq j.$$  \[A9\]

**APPENDIX B**

This Appendix outlines proof of the mutual orthogonality of the three tensor invariants that comprise the two possible sets described under Theory, namely the set composed of $\mathbf{tr}(\mathbf{A})$, $\mathbf{norm}(\mathbf{A})$, and $\mathbf{mode}(\mathbf{A})$ and the set composed of $\mathbf{norm}(\mathbf{A})$, $\mathbf{FA}(\mathbf{A})$, and $\mathbf{mode}(\mathbf{A})$. Recall, the anisotropic part of tensor $\mathbf{A}$ is denoted $\tilde{\mathbf{A}}$ as defined in Eq. [5].

**Mutual Orthogonality of $K_1$, $K_2$, and $K_3$**

The following extended definitions of Eqs. [6–8] are essential for the proofs that follow and are all found in the work of Criscione et al. (6).

$$K_1 = \mathbf{tr}(\mathbf{A}) = \mathbf{I}:\mathbf{A}$$  \[B1\]

$$K_2 = \mathbf{norm}(\mathbf{\tilde{A}}) = \sqrt{\mathbf{\tilde{A}}:\mathbf{\tilde{A}}} = \mathbf{\Phi} : \mathbf{A}$$  \[B2\]

$$K_3 = \mathbf{mode}(\mathbf{\tilde{A}}) = 3 \sqrt{6} \det(\mathbf{\Phi}) = \sqrt{6} (\Phi^2 : \mathbf{I}) = \sqrt{6} (\Phi^2 : \mathbf{\Phi})$$  \[B3\]

The tensor $\mathbf{\Phi}$ (defined in Eq. [11]) is symmetric, anisotropic, and has the following useful properties:

$$\mathbf{\Phi} : \mathbf{\Phi} = \mathbf{\Phi}^2 : \mathbf{I} = \mathbf{tr}(\mathbf{\Phi}^2) = 1,$$  \[B4\]

$$\mathbf{\Phi} : \mathbf{I} = \mathbf{tr}(\mathbf{\Phi}) = 0.$$  \[B5\]

Note that Eq. [B4] is true by definition as $\mathbf{\Phi}$ is defined as a normalized tensor and that Eq. [B5] will be subject to a proof in this Appendix. Furthermore, variation of Eqs. [B4] and [B5] using the Chain Rule provides two useful identities for the proofs that follow:

$$\partial \mathbf{\Phi} : \mathbf{\Phi} = 0$$  \[B6\]

$$\partial \mathbf{\Phi} : \mathbf{I} = 0$$  \[B7\]

**Proof of Mutual Orthogonality of $K_1$–$K_3$ Gradients**

To define the gradient of $K_i$ increment Eq. [B1] using the Chain Rule to obtain $\partial K_1 = \mathbf{I}:d\mathbf{A}$ (recall $d\mathbf{I} = 0$). Hence, by Eq. [A8] we can define the gradient of $K_i$ as

$$\frac{\partial K_1}{\partial \mathbf{A}} = \mathbf{I}.$$  \[B8\]

To determine the gradient of $K_2$, take the variation of [B2] to obtain $\partial K_2 = \partial (\mathbf{\Phi} : \mathbf{A}) + \mathbf{\Phi} : d\mathbf{A}$. Substituting into this expression those found in Eqs. [10], [B6], and [B7] we obtain

$$dK_2 = d \mathbf{norm}(\mathbf{\tilde{A}}) = \mathbf{\Phi} : d\mathbf{A}.$$  \[B9\]

Thus, the gradient of $K_2$ is

$$\frac{\partial K_2}{\partial \mathbf{A}} = \mathbf{\Phi}.$$  \[B10\]

Taking the variation of Eq. [B3] results in $dK_3 = 3 \sqrt{6} (\Phi^2 : \mathbf{\Phi})$ after applying Eq. [A6] and $d\mathbf{I} = 0$. If we take the variation of Eq. [10] and solve for $\partial \mathbf{\Phi}$, recalling that $dK_1 = \mathbf{I}:d\mathbf{A}$ and Eq. [B9] we obtain $\partial \mathbf{\Phi} = K_2^{-1}(d\mathbf{A} - \frac{1}{3} [\mathbf{I} : d\mathbf{A}] \mathbf{I} - (\mathbf{\Phi} : d\mathbf{A}) \mathbf{\Phi})$, which can be used to recast $dK_3$ using Eqs. [B3] and [B4] to show that

$$dK_3 = \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_2 \Phi - \sqrt{6} \mathbf{I}) : d\mathbf{A}.$$  \[B11\]

Thus, we can define the gradient of $K_3$ as

$$\frac{\partial K_3}{\partial \mathbf{A}} = \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_2 \Phi - \sqrt{6} \mathbf{I}).$$  \[B12\]

Proving that $\frac{\partial K_1}{\partial \mathbf{A}}$ and $\frac{\partial K_2}{\partial \mathbf{A}}$ are mutually orthogonal is straightforward. The orthogonality of $K_1$ and $K_2$ requires proving that $\frac{\partial K_1}{\partial \mathbf{A}} : \frac{\partial K_2}{\partial \mathbf{A}} = 0$. From Eqs. [B8] and [B10] we know that

$$\frac{\partial K_1}{\partial \mathbf{A}} : \frac{\partial K_2}{\partial \mathbf{A}} = \mathbf{\Phi} : \mathbf{\Phi} = 0.$$  \[B13\]


$$\frac{\partial K_1}{\partial \mathbf{A}} : \frac{\partial K_2}{\partial \mathbf{A}} = \mathbf{\Phi} : \mathbf{\Phi} \mathbf{\Phi}^{-1} ([\mathbf{I} : \mathbf{A}]) - \frac{1}{3} ([\mathbf{I} : \mathbf{A}] : \mathbf{I}) \mathbf{I}.$$  \[B14\]

This expression is reduced to zero with $\mathbf{I} : \mathbf{I} = 3$; therefore,

$$\frac{\partial K_1}{\partial \mathbf{A}} : \frac{\partial K_2}{\partial \mathbf{A}} = 0.$$  \[B15\]

Proving the orthogonality of $K_2$ and $K_3$ requires showing that $\frac{\partial K_2}{\partial \mathbf{A}} : \frac{\partial K_3}{\partial \mathbf{A}} = 0$. With Eqs. [B10] and [B12], we have

$$\frac{\partial K_2}{\partial \mathbf{A}} : \frac{\partial K_3}{\partial \mathbf{A}} = \mathbf{\Phi} : \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_2 \Phi - \sqrt{6} \mathbf{I}).$$  \[B16\]

Use of Eq. [A2] and substitution of Eqs. [B3–B5] provides
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\[
\frac{\partial K_2}{\partial A} : \frac{\partial K_3}{\partial A} = \frac{1}{K_2} (3 \sqrt{6} K_3 - 3 K_3), \quad [B17]
\]

which reduces to

\[
\frac{\partial K_3}{\partial A} : \frac{\partial K_3}{\partial A} = 0. \quad [B18]
\]

Proving the orthogonality of \(K_1\) and \(K_3\) requires showing that \(\frac{\partial K_1}{\partial A} : \frac{\partial K_1}{\partial A} = 0\). From Eqs. [B8] and [B12] we have

\[
\frac{\partial K_3}{\partial A} : \frac{\partial K_1}{\partial A} = \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_3 \Phi - \sqrt{6} I). \quad [B19]
\]

Use of Eq. [A2], substitution of Eqs. [B4] and [B5], and recalling \(I I = 3\) results in

\[
\frac{\partial K_3}{\partial A} : \frac{\partial K_1}{\partial A} = \frac{1}{K_2} (3 \sqrt{6} - 0 - \sqrt{6}(3)). \quad [B20]
\]

This clearly reduces to

\[
\frac{\partial K_3}{\partial A} : \frac{\partial K_1}{\partial A} = 0. \quad [B21]
\]

With Eqs. [B15], [B18], and [B21] it is clear that the gradients of \(K_1K_3\) form a mutually orthogonal set.

Proof of Mutual Orthogonality of \(R_1-R_3\) Gradients

The second set of orthogonal tensor invariants was described under Theory and is summarized below.

\[
R_1 = \text{norm}(A) = \sqrt{\text{det}(A)} \quad [B22]
\]

\[
R_2 = FA(A) = \sqrt[3]{2} \frac{\text{norm}(\bar{A})}{\text{norm}(A)} \quad [B23]
\]

\[
R_3 = \text{mode}(A) = 3 \sqrt{6} \text{ det}(\Phi) \quad [B24]
\]

To define the gradient of \(R_1\), we take the variation of Eq. [B22] using the Chain Rule,

\[
dR_1 = d\text{norm}(A) = \frac{1}{2} \left( A : A \right)^{-1/2} (dA : A + A : dA). \quad [B25]
\]

This can be simplified using Eq. [A3] to show that the gradient of \(R_1\) is

\[
\frac{\partial R_1}{\partial A} = \text{norm}(A)^{-1} A. \quad [B26]
\]

To define the gradient of \(R_2\) we begin by taking its variation using the quotient rule,

\[
dR_2 = dFA = \sqrt{\frac{3}{2}} \frac{\text{norm}(A) d\text{norm}(\bar{A}) - \text{norm}(\bar{A}) d \text{norm}(A)}{\text{norm}(A)^2}. \quad [B27]
\]

Substitution of Eqs. [B9] and [B25] into Eq. [B27] results in the following:

\[
dR_2 = dFA = \sqrt{\frac{3}{2}} \frac{1}{\text{norm}(A)^2} \left( \text{norm}(A) \Phi - \text{norm}(\bar{A}) \text{norm}(A)^{-1} A \right) : dA. \quad [B28]
\]

Thus, the gradient of \(R_2\) is

\[
\frac{\partial R_2}{\partial A} = \sqrt{\frac{3}{2}} \left( \frac{1}{\text{norm}(A)} \Phi - \text{norm}(\bar{A}) \text{norm}(A)^{-1} A \right). \quad [B29]
\]

The gradient of \(R_3\) is equivalent to the gradient of \(K_3\); hence from Eq. [B19],

\[
\frac{\partial R_3}{\partial A} = \frac{\partial K_3}{\partial A} = \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_3 \Phi - \sqrt{6} I). \quad [B30]
\]

To prove that the gradient of \(R_3\) is orthogonal to the gradient of \(R_2\), contract Eqs. [B26] and [B29],

\[
\frac{\partial R_1}{\partial A} : \frac{\partial R_2}{\partial A} = \frac{\partial K_3}{\partial A} = \frac{3}{2} \left( A : \Phi - \text{norm}(\bar{A}) \text{norm}(A)^{-1} (A:A) \right). \quad [B31]
\]

Substitution of Eqs. [2] and [B2] in Eq. [B31] results in the following after simplification:

\[
\frac{\partial R_1}{\partial A} : \frac{\partial R_2}{\partial A} = 0 \quad [B32]
\]

To prove the orthogonality of the gradients of \(R_2\) and \(R_3\), it is useful to define the contraction of \(A\) and \(\Phi^2\) by combining Eqs. [10], [B3], and [B4] to find

\[
A : \Phi^2 = \frac{1}{2} K_1 + K_3 K_3 / \sqrt{6}. \quad [B33]
\]

The contraction of Eqs. [B29] and [B30] has the following form,

\[
\frac{\partial R_1}{\partial A} : \frac{\partial R_2}{\partial A} = \left( \sqrt{\frac{3}{2}} \left( \frac{1}{\text{norm}(A)} \Phi - \text{norm}(\bar{A}) \text{norm}(A)^{-1} A \right) : \right)
\]

\[
\left( \frac{1}{K_2} (3 \sqrt{6} \Phi^2 - 3 K_3 \Phi - \sqrt{6} I) \right), \quad [B34]
\]

and application of Eq. [A2] results in a lengthy expansion,

\[
\frac{\partial R_1}{\partial A} : \frac{\partial R_2}{\partial A} = \sqrt{\frac{3}{2}} \frac{1}{K_2} \left( \text{norm}(A)^{-1} (3 \sqrt{6} \Phi^2 - 3 K_3 \Phi - \sqrt{6} I) \right) - \frac{\text{norm}(\bar{A})}{\text{norm}(A)^3} (3 \sqrt{6} A : \Phi^2 - 3 K_3 A : \Phi - \sqrt{6} A : I), \quad [B35]
\]

which is simplified upon substitution of Eqs. [B1–B5] and [B33].
\[
\frac{\partial R_2}{\partial \mathbf{A}} : \frac{\partial R_3}{\partial \mathbf{A}} = \sqrt{\frac{3}{2}} \left( \text{norm}(\mathbf{A})^{-1} \left[ 3 \sqrt{6} (K_3/\sqrt{6}) - 3K_1 \right] - \frac{\text{norm}(\mathbf{\hat{A}})}{\text{norm}(\mathbf{A})} \left[ 3 \sqrt{6} (K_3/\sqrt{6}) - 3K_2 \right] \right).
\]

After the use of Eq. [A2] and substitution of Eqs. [B38], [B39], and [B40] we arrive at

\[
\frac{\partial \text{tr}(\mathbf{A})}{\partial \mathbf{A}} : \frac{\partial \text{FA}(\mathbf{A})}{\partial \mathbf{A}} = I : \sqrt{\frac{3}{2}} \left( \frac{1}{\text{norm}(\mathbf{A})} \Phi - \frac{\text{norm}(\mathbf{\hat{A}})}{\text{norm}(\mathbf{A})} \mathbf{A} \right).
\]

Thus, it can be seen that the gradients of \(K_3\) and \(R_3\) are not orthogonal. It is interesting to note, however, that the gradients approach being orthogonal as the tensor trace or fractional anisotropy decreases. Hence, \(K_1\) and \(R_2\) are nearly orthogonal for low anisotropy.

**REFERENCES**