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Principal invariants and inherent parameters of diffusion kurtosis tensors ${}^{\bigstar}$

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ABSTRACT

A diffusion kurtosis (DK) tensor is a fourth order three-dimensional fully symmetric tensor, which is used in diffusion kurtosis imaging (DKI), a new model in medical engineering. To understand the biological and clinical meaning of the DK tensor, we have to measure and calculate some quantities and parameters which are independent from coordinate system choices. In this paper we study such quantities and parameters. They include the largest, the smallest and the average apparent kurtosis coefficients (AKC) values, which are invariant from the coordinate system choices, and some parameters measured in the inherent coordinate system, which is formed by the eigenvector system of the second order diffusion tensor. We study their computational formulas and relationships.

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1. Introduction

Diffusion magnetic resonance imaging (D-MRI) has been developed in biomedical engineering for decades. It measures the apparent diffusivity of water molecules in human or animal tissues, such as brain and blood, to acquire biological and clinical information. In tissues, such as brain gray matter, where the measured apparent diffusivity is largely independent of the orientation of the tissue (i.e., isotropic), it is usually sufficient to characterize the diffusion characteristics with a single (scalar) apparent diffusion coefficient (ADC). However, in anisotropic media, such as skeletal and cardiac muscle and in white matter, where the measured diffusivity is known to depend upon the orientation of the tissue, no single ADC can characterize the orientation-dependent water mobility in these tissues. Because of this, a diffusion tensor model was proposed years ago to replace the diffusion scalar model. This resulted in diffusion tensor imaging (DTI).

A diffusion tensor *D* is a second order three-dimensional positive definite symmetric tensor. Under a Cartesian laboratory coordinate system, it is represented by a real three-dimensional symmetric matrix, which has six independent elements $D = (D_{ij})$ with $D_{ij} = D_{ji}$ for i, j = 1, 2, 3. There is a relationship

$$\ln[S(b)] = \ln[S(0)] - bD_{app}.$$
(1)

Here S(b) is the signal intensity at the echo time, D_{app} is the ADC value at the direction x,

$$D_{\text{app}} = \sum_{i,j=1}^{3} D_{ij} x_i x_j, \tag{2}$$

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⁰⁰²²⁻²⁴⁷X/\$ – see front matter $\,\, @$ 2008 Elsevier Inc. All rights reserved. doi:10.1016/j.jmaa.2008.08.049 $\,$

 $x = (x_1, x_2, x_3)$ is the unit direction vector, satisfying $\sum_{i=1}^{3} x_i^2 = 1$, the parameter *b* is given by

$$b = (\gamma \, \delta g)^2 \left(\Delta - \frac{\delta}{3} \right),$$

g is the gradient strength, γ is the proton gyromagnetic ratio, Δ is the separation time of the two diffusion gradients, δ is the duration of each gradient lobe [8].

Combining (1) and (2), we have

$$\ln[S(b)] = \ln[S(0)] - \sum_{i,j=1}^{3} bD_{ij}x_ix_j.$$
(3)

There are six unknown variables D_{ij} in the formula (3). By applying the magnetic gradients in six or more non-collinear, non-coplanar directions, one can solve (3) and get the six independent elements D_{ij} . Let the eigenvalues of D be $\alpha_1 \ge \alpha_2 \ge \alpha_3 > 0$. Then the mean diffusivity [2] can be calculated by

$$M_D = \frac{\alpha_1 + \alpha_2 + \alpha_3}{3},$$

while the fractional anisotropy [2] is

$$FA = \sqrt{\frac{3}{2}} \sqrt{\frac{(\alpha_1 - M_D)^2 + (\alpha_2 - M_D)^2 + (\alpha_3 - M_D)^2}{\alpha_1^2 + \alpha_2^2 + \alpha_3^2}}$$

where $0 \le FA \le 1$. If FA = 0, the diffusion is isotropic. If FA = 1, the diffusion is anisotropic. Since the eigenvalues of D are invariants with respect to coordinate system rotation, M_D and FA are also invariants of D. They can be used for biological and clinical analysis.

The diffusion tensor imaging model (DTI) is now used widely in biological and clinical research [2,6,9]. However, DTI is known to have a limited capability in resolving multiple fibre orientations within one voxel [1,10,16]. This is mainly because the probability density function for random spin displacement is non-Gaussian in the confining environment of biological tissues and, thus, the modelling of self-diffusion by a second order tensor breaks down. Recently, a new MRI model is presented in [8,11].

The authors of [8,11] propose to use a fourth order three-dimensional fully symmetric tensor, called the diffusion kurtosis (DK) tensor, to describe the non-Gaussian behavior. The values of the fifteen independent elements of the DK tensor *W* can be obtained by the MRI technique. The diffusion kurtosis imaging (DKI) has important biological and clinical significance.

A diffusion kurtosis tensor W is a fourth order three-dimensional fully symmetric tensor. Under a Cartesian laboratory coordinate system, it is represented by a real fourth order three-dimensional fully symmetric array, which has fifteen independent elements $W = (W_{ijkl})$ with W_{ijkl} being invariant for any permutation of its indices i, j, k, l = 1, 2, 3. The relationship (1) can be further expanded (adding a second order Taylor expansion term on b) to (see [8,11], for example):

$$\ln[S(b)] = \ln[S(0)] - bD_{app} + \frac{1}{6}b^2 D_{app}^2 K_{app},$$
(4)

where K_{app} is the apparent kurtosis coefficient (AKC) value at the direction x (see [8,11], for example),

$$D_{\rm app}^2 K_{\rm app} = M_D^2 \sum_{i,j,k,l=1}^3 W_{ijkl} x_i x_j x_k x_l.$$
(5)

Combining (4), (2) and (5), we have

$$\ln[S(b)] = \ln[S(0)] - \sum_{i,j=1}^{3} bD_{ij}x_ix_j + \frac{1}{6}b^2M_D^2 \sum_{i,j,k,l=1}^{3} W_{ijkl}x_ix_jx_kx_l.$$
(6)

The non-Gaussian behavior of water molecules may contain useful information related to tissue structure and pathophysiology. Hence, the diffusion kurtosis imaging (DKI) has important biological and clinical significance. The authors of [8,11] found sharp differences between the diffusion kurtosis in white and gray matters. They believe that DKI is potentially of value for the assessment of neurologic diseases, such as multiple sclerosis and epilepsy, with associated white matter abnormalities. Additional, DKI may be useful for investigating abnormalities in tissues with isotropic structures, such as gray matter, where techniques like DTI are less applicable. This is supported by the results in many experimental studies of DKI, where the diffusion kurtosis is not zero, while DTI models treat it as zero.

The values of the fifteen independent elements of the DK tensor W can be obtained with the six independent elements of the diffusion tensor D together by the MRI technique and the least squares method, as suggested in [8,11]. However, these values are not independent of the coordinate system. When the coordinate system is rotated, these values will be changed. To understand the biological and clinical meaning of the DK tensor, a mathematical study on invariants of the DK tensor

is necessary. In [20], Qi, Wang and Wu introduced *D-eigenvalues* for a DK tensor. It was shown that the D-eigenvalues of a DK tensor are invariants of the DK tensor. The largest and the smallest D-eigenvalues of a DK tensor correspond with the largest and the smallest AKC values of a water molecule in the space, respectively. A computational method for calculating D-eigenvalues of a DK tensor was also presented in [20]. The concept of D-eigenvalues is an extension of the Z-eigenvalues introduced in [17] and studied in [15,18,19].

In the literature, there are some other "eigenvalues" for a fourth order fully symmetric tensor. In particular, Lord Kelvin [21,22] introduced such eigenvalues, also see [3,14]. We call them *Kelvin eigenvalues*. The calculation of the Kelvin eigenvalues is much easier, since they are actually eigenvalues of a 6×6 symmetric matrix. However, the definition of D-eigenvalues is closer to the formula (5) of AKC values than the definition of Kevin eigenvalues. In Section 2, we will explain this point.

The largest and the smallest AKC values are two important invariants of a DK tensor. Apart from them, there are other important invariants of a DK tensor. For example, the spherical average AKC value should be another important invariant of the DK tensor. We study the computational formulas and properties of this quantity in Section 3. We show that it is a linear function of the diagonal and sub-diagonal elements of the DK tensor.

It is well known that the eigenvector system of the second order diffusion tensor forms a Cartesian coordinate system. The eigenvector associated with the largest eigenvalue of the diffusion tensor is parallel to the direction of the dominant tissue structure (such as white matter fiber along which the water molecules diffuse the most), while the eigenvectors associated with the other two eigenvalues are perpendicular to the direction of the dominant tissue structure. Hence, this coordinate system has its physical meanings. We call this coordinate system *the inherent coordinate system* of the DK tensor. Since this coordinate system is not arbitrary, the form of the DK tensor under this system should have some physical meanings too. In Section 4, we study the computational formulas of this special form of the DK tensor, and the average AKC value over the characteristic ellipsoidal surface of the ADC values. We call this average AKC value the ellipsoidal average AKC value, which is a kind of weighted average AKC values. We show that it is a linear function of the diagonal and sub-diagonal elements of the form of the DK tensor in the inherent coordinate system. The AKC values along the coordinate directions of the inherent coordinate system were studied in [7].

The coefficients of the linear functions of the spherical and the ellipsoidal AKC values involve surface integrals over the spherical and the ellipsoidal surfaces. In Section 5, we use the eigenvalues of the diffusion tensor to scale the inherent coordinate system to smooth the characteristic ellipsoidal surface of the ADC values to a spherical surface. Then, we find that the average AKC value over this surface is equal to one fifth of the sum of the diagonal elements plus two fifths of the sum of the sub-diagonal elements of the form of the DK tensor in the scaled inherent coordinate system. We show that this value is equal to one fifth of the sum of the special form of the DK tensor. We then show that all the AKC values are bounded by the largest and the smallest Kelvin eigenvalues of this special form, but there are gaps between the largest/smallest Kelvin eigenvalue and the largest/smallest AKC value. This further justifies the significance of D-eigenvalues.

In Section 6, we provide two numerical examples and five maps which are based upon the magnetic resonance diffusion data acquired out of rat spinal cord samples. Some final remarks are made in Section 7. To make the paper self-contained, we include an appendix as Section 8 on the calculation of D-eigenvalues and D-eigenvectors.

2. D-eigenvalues and Kelvin eigenvalues

We use $x = (x_1, x_2, x_3)^T$ to denote the direction vector, which is denoted as $n = (n_1, n_2, n_3)^T$ in [8,11].

As described in [8,11], the ADC and AKC values for a single direction can be determined by acquiring data at three or more *b* values (including b = 0) and fitting to Eq. (4). Then, by solving the resulted nonlinear system via, for example, the least-squares method, the apparent diffusion coefficient D_{app} and the apparent kurtosis coefficient K_{app} for the given direction can be obtained.

As noted in the introduction, *W* is a fourth order three-dimensional fully symmetric tensor. Hence, *W* has 15 independent elements. For those elements of *W* which are equal to each other because of symmetry, we use the element W_{ijkl} with $i \leq j \leq k \leq l$ to represent them. So if we say that $W_{1122} = 3$, this automatically implies that $W_{1212} = W_{2112} = W_{2121} = W_{1221} = W_{2211} = 3$. Then, the 15 independent elements of *W* are W_{1111} , W_{2222} , W_{3333} , W_{1122} , W_{1133} , W_{2233} , W_{1123} , W_{1223} , W_{1233} , W_{1223} , W_{1233} , W_{1223} , W_{1233} , W_{1223} , W_{1233} , W_{1223} , W_{1333} , W_{2233} the sub-diagonal elements of *W*.

Denote the largest and the smallest AKC values as K_{max} and K_{min} respectively. By [20],

$$K_{\max} = \max M_D^2 \sum_{\substack{i,j,k,l=1\\i,j=1}}^3 W_{ijkl} x_i x_j x_k x_l$$

s.t.
$$\sum_{\substack{i,j=1\\i,j=1}}^3 D_{ij} x_i x_j = 1,$$

and

(7)

$$K_{\min} = \min M_D^2 \sum_{i,j,k,l=1}^{3} W_{ijkl} x_i x_j x_k x_l$$

s.t. $\sum_{i,j=1}^{3} D_{ij} x_i x_j = 1.$ (8)

The critical points of the maximization problem (7) and the minimization problem (8) satisfy the following system for some $\lambda \in \Re$ and $x \in \Re^3$:

$$\begin{cases} \sum_{j,k,l=1}^{3} W_{ijkl} x_j x_k x_l = \lambda \sum_{j=1}^{3} D_{ij} x_j, & i = 1, 2, 3, \\ \sum_{i,j=1}^{3} D_{ij} x_i x_j = 1. \end{cases}$$
(9)

A real number λ satisfying (9) with a real vector x is called a *D*-eigenvalue of W, and the real vector x is called the *D*-eigenvector of W associated with the D-eigenvalue λ . Since D-eigenvectors are critical points of the maximization problem (7) and the minimization problem (8), by the theory of optimization, they are local maximizers, local minimizers and saddle points of the optimization problems (7) and (8), while D-eigenvalues are corresponding Lagrangian multipliers. These are the geometrical meanings of D-eigenvalues and D-eigenvectors. The following two theorems are proved in [20].

Theorem 1. *D*-eigenvalues are real numbers and always exist. If x is a D-eigenvector associated with a D-eigenvalue λ , then

$$\lambda = \sum_{i,j,k,l=1}^{3} W_{ijkl} x_i x_j x_k x_l.$$

Denote the largest and the smallest D-eigenvalues of W as λ_{max} and λ_{min} respectively. Then

$$K_{\rm max} = M_D^2 \lambda_{\rm max},\tag{10}$$

and

$$K_{\min} = M_D^2 \lambda_{\min}.$$
 (11)

Theorem 2. The D-eigenvalues of W are invariant under rotations of coordinate systems.

By these two theorems, K_{max} and K_{min} are also invariants of W. Computational formulas were given in [20] for calculating D-eigenvalues. Hence, we may calculate K_{max} and K_{min} by the method given in [20].

We now discuss Kelvin eigenvalues of W. Let X be a second order three-dimensional symmetric tensor with elements X_{ij} . Define WX as another second order symmetric tensor with its elements as

$$(WX)_{ij} = \sum_{k,l=1}^{3} W_{ijkl} X_{kl}.$$

If a number μ and a nonzero second order symmetric tensor X satisfy

 $WX = \mu X$,

then we say that μ is a *Kelvin eigenvalue* of W and X is an *eigentensor* of W associated with the Kelvin eigenvalue μ . There is an isomorphism between the Kelvin eigenvalues and eigentensors of W, and the eigenvalues and eigenvectors

of the six-dimensional symmetric matrix

	(W ₁₁₁₁	W_{1122}	W_{1133}	$\sqrt{2W_{1112}}$	$\sqrt{2W_{1113}}$	$\sqrt{2W_{1123}}$
U =	W ₁₁₂₂	W_{2222}	W ₂₂₃₃	$\sqrt{2}W_{1222}$	$\sqrt{2}W_{1223}$	$\sqrt{2}W_{2223}$
	W ₁₁₃₃	W ₂₂₃₃	W ₃₃₃₃	$\sqrt{2}W_{1233}$	$\sqrt{2}W_{1333}$	$\sqrt{2}W_{2333}$
	$\sqrt{2}W_{1112}$	$\sqrt{2}W_{1222}$	$\sqrt{2}W_{1233}$	$2W_{1122}$	$2W_{1123}$	2W ₁₂₂₃
	$\sqrt{2}W_{1113}$	$\sqrt{2}W_{1223}$	$\sqrt{2}W_{1333}$	$2W_{1123}$	$2W_{1133}$	2W ₁₂₃₃
	$\sqrt{2}W_{1123}$	$\sqrt{2}W_{2223}$	$\sqrt{2}W_{2333}$	$2W_{1223}$	$2W_{1233}$	2W ₂₂₃₃ /

Thus, the six Kelvin eigenvalues of *W* are all real. If *X* is an eigentensor of *W*, associated with a Kelvin eigenvalue μ of *W*, then the vector $(X_{11}, X_{22}, X_{33}, \sqrt{2}X_{12}, \sqrt{2}X_{13}, \sqrt{2}X_{23})^T$ is an eigenvector of *U* associated with the eigenvalue μ of *U*. See [3].

It is easy to see that Kelvin eigenvalues of W are also invariants of W. They are much easier to be calculated as they are actually eigenvalues of the matrix U. However, it can be shown that they are less close to the largest and the smallest AKC values. Let the largest and the smallest Kelvin eigenvalues of W be μ_{max} and μ_{min} respectively, we have

$$\mu_{\max} = \max \sum_{i,j,k,l=1}^{3} W_{ijkl} X_{ij} X_{kl}$$

s.t.
$$\sum_{i,j=1}^{3} X_{ij}^{2} = 1,$$
 (12)

and

$$\mu_{\min} = \min \sum_{i,j,k,l=1}^{3} W_{ijkl} X_{ij} X_{kl}$$

s.t.
$$\sum_{i,j=1}^{3} X_{ij}^{2} = 1.$$
 (13)

The optimization problems (12) and (13) are matrix optimization problems as their optimization variables are the matrix $X = (X_{ij})$. Comparing (12) and (13) with (7) and (8), we see that D-eigenvalues reflect more the extremal AKC values than Kelvin eigenvalues. Suppose that we have a feasible solution x for (7) and (8). Let $X_{ij} = x_i x_j$ for i, j = 1, 2, 3. Then we have a feasible solution x for (7) and (8). Let $X_{ij} = x_i x_j$ for i, j = 1, 2, 3. Then we have a feasible solution x for (7) and (12) and (13). On the other hand, a feasible solution X of (12) and (13) does not produce a feasible solution x for (7) and (8), unless the rank of the matrix X is one. Thus, the feasible set of (12) and (13) is larger and includes feasible solutions X which cannot be decomposed as $X_{ij} = x_i x_j$ for i, j = 1, 2, 3 for some x. Hence, we cannot use Kelvin eigenvalues to represent the largest and the smallest AKC values. This justifies the significance of D-eigenvalues.

3. The spherical average AKC value

Denote the unit sphere as

$$S := \{ x \in \mathfrak{R}^3 \colon x_1^2 + x_2^2 + x_3^2 = 1 \}.$$

Then the spherical average AKC value is defined as

$$M_{S} = \frac{1}{S} \iint_{S} K_{\text{app}} dA = \frac{M_{D}^{2}}{4\pi} \iint_{S} \frac{\sum_{i,j,k,l=1}^{3} W_{ijkl} x_{i} x_{j} x_{k} x_{l}}{\left(\sum_{i,j=1}^{3} D_{ij} x_{i} x_{j}\right)^{2}} dA,$$
(14)

where the denominator $S = 4\pi$ is the area of the surface *S*. Here, we slightly abuse the symbol *S* for both the surface and its area.

Theorem 3. We have

$$K_{\min} \leqslant M_S \leqslant K_{\max}.$$
 (15)

The quantity M_S is invariant under rotation of coordinate systems. It is a linear function of the diagonal and sub-diagonal elements of W. It is also invariant if D is scaled, i.e., if D is changed to βD and W has no change, where β is a positive number, then M_S has no change.

Proof. Formula (15) follows from (14) directly. The surface *S* is independent from rotations of coordinate systems. Hence M_S is invariant under rotations of coordinate systems. By the definitions of M_S as well as the symmetry of the elements of W, we have its computational formulas as follows.

$$M_{S} = \frac{M_{D}^{2}}{4\pi} [A_{1}W_{1111} + A_{2}W_{2222} + A_{3}W_{3333} + 4A_{4}W_{1112} + 4A_{5}W_{1113} + 4A_{6}W_{1222} + 4A_{7}W_{2223} + 4A_{8}W_{1333} + 4A_{9}W_{2333} + 6A_{10}W_{1122} + 6A_{11}W_{1133} + 6A_{12}W_{2233} + 12A_{13}W_{1123} + 12A_{14}W_{1223} + 12A_{15}W_{1233}],$$

where

A

$$A_i = \iint_{S} \frac{a_i(x)}{\left(\sum_{i,j=1}^{3} D_{ij} x_i x_j\right)^2} dA$$

with $a_1(x) = x_1^4$, $a_2(x) = x_2^4$, $a_3(x) = x_3^4$, $a_4(x) = x_1^3x_2$, $a_5(x) = x_1^3x_3$, $a_6(x) = x_1x_2^3$, $a_7(x) = x_2^3x_3$, $a_8(x) = x_1x_3^3$, $a_9(x) = x_2x_2^3$, $a_{10}(x) = x_1^2x_2^2$, $a_{11}(x) = x_1^2x_3^2$, $a_{12}(x) = x_2^2x_3^2$, $a_{13}(x) = x_1^2x_2x_3$, $a_{14}(x) = x_1x_2^2x_3$ and $a_{15}(x) = x_1x_2x_3^2$. By symmetry, we see that $A_i = 0$ for i = 4, ..., 9 and i = 13, 14, 15, These show that M_5 is a linear function of the diagonal and sub-diagonal elements of W.

Let *D* be changed to βD , where β is a positive number. In (14), M_D^2 will be changed to $\beta^2 M_D^2$ and the denominator of the fraction will be multiplied by β^2 . Then M_S is not changed. The theorem is proved. \Box

The coefficients A_i cannot be computed exactly in general. But they can be computed numerically. For the integral over S, we may use the parametric expression

$$x = \begin{pmatrix} \cos\theta\sin\phi\\ \sin\theta\sin\phi\\ \cos\phi \end{pmatrix}$$

for *S*, where $0 \leq \theta < 2\pi$, $0 \leq \phi \leq \pi$. Then

$$\iint_{S} f(x) dA = \int_{0}^{2\pi} \int_{0}^{\pi} f(\cos\theta\sin\phi, \sin\theta\sin\phi, \cos\phi) \sin\phi d\phi d\theta.$$

4. The inherent coordinate system and the ellipsoidal average AKC value

We may make an orthogonal transformation to the coordinate system such that the three orthonormal eigenvectors of D are used as the coordinate base vectors. As we said in the introduction, this coordinate system has its own physical meaning and is fixed when D is fixed. We call this coordinate system the inherent coordinate system of W, and call the form of D and W in this coordinate system the *inherent forms* of D and W respectively.

Let the columns of an orthogonal matrix *P* consist of three orthonormal eigenvectors of *D*. Denote $P = (p_{ij})$. Let *x* be converted to y = Px. Then *D* and *W* are converted to their inherent forms \hat{D} and \hat{W} , where the elements of \hat{D} and \hat{W} are defined by

$$\hat{D}_{ij} = \sum_{i',j'=1}^{3} D_{i'j'} p_{i'i} p_{j'j},$$

and

$$\hat{W}_{ijkl} = \sum_{i', j', k', l'=1}^{3} W_{i'j'k'l'} p_{i'i} p_{j'j} p_{k'k} p_{l'l}$$

respectively, see [17] for the definition of orthogonal similarity. By the knowledge of linear algebra, we know that P, as an orthogonal matrix, either is a rotation matrix, or the product of a rotation matrix and a reflection matrix, depending upon the system of the orthonormal eigenvectors of D are right-handed or left-handed. Then, since the columns of P consist of three orthonormal eigenvectors of D, \hat{D} is a diagonal matrix with the eigenvalues of D as its diagonal elements, i.e.,

$$\hat{D} = \begin{pmatrix} \alpha_1 & 0 & 0 \\ 0 & \alpha_2 & 0 \\ 0 & 0 & \alpha_3 \end{pmatrix}.$$

The elements \hat{W}_{iikl} have their own physical meanings. By (5), we have the following theorem.

Theorem 4. The AKC value along the direction of the eigenvector associated with the eigenvalue α_i of D for i = 1, 2, 3, is

$$K_i = \frac{M_D^2}{\alpha_i^2} \hat{W}_{iiii}.$$

Thus, K_i for i = 1, 2, 3, along with K_{max} , K_{min} , and K_S , form important reference quantities of W. Since K_i , for i = 1, 2, 3, are calculated on the inherent coordinate system, we call them and the other quantities discussed in the latter part of our paper as *inherent parameters*. For some further discussions on K_i for i = 1, 2, 3, see [7].

We now consider the average AKC value over the characteristic ellipsoid surface of ADC:

$$S_E := \{ y \in \mathfrak{N}^3 \colon \hat{D}y^2 = 1 \} = \{ y \in \mathfrak{N}^3 \colon \alpha_1 y_1^2 + \alpha_2 y_2^2 + \alpha_3 y_3^2 = 1 \}.$$

Then the ellipsoidal average AKC value is defined as

$$M_{E} = \frac{1}{S_{E}} \iint_{S_{E}} K_{app} dA = \frac{M_{D}^{2}}{S_{E}} \iint_{S_{E}} \sum_{i,j,k,l=1}^{3} \hat{W}_{ijkl} y_{i} y_{j} y_{k} y_{l} dA,$$
(16)

where the denominator S_E is the area of the surface S_E ,

$$S_E = \iint_{S_E} dA.$$

Again, we use the symbol S_E for both the surface and its area.

Theorem 5. We have

$$K_{\min} \leqslant M_E \leqslant K_{\max}.$$
(17)

The quantity M_E is a linear function of the diagonal and sub-diagonal elements of \hat{W} . It is also invariant if D is scaled, i.e., if D is changed to βD and W has no change, where β is a positive number, then M_E has no change.

Proof. The formula (17) follows from (16) directly. By the definition of M_E as well as the symmetry of the elements of W, we have its computational formulas as follows.

$$M_E = \frac{M_D^2}{S_E} [B_1 \hat{W}_{1111} + B_2 \hat{W}_{2222} + B_3 \hat{W}_{3333} + 4B_4 \hat{W}_{1112} + 4B_5 \hat{W}_{1113} + 4B_6 \hat{W}_{1222} + 4B_7 \hat{W}_{2223} + 4B_8 \hat{W}_{1333} + 4B_9 \hat{W}_{2333} + 6B_{10} \hat{W}_{1122} + 6B_{11} \hat{W}_{1133} + 6B_{12} \hat{W}_{2233} + 12B_{13} \hat{W}_{1123} + 12B_{14} \hat{W}_{1223} + 12B_{15} \hat{W}_{1233}],$$

where

$$B_i = \iint_{S_E} b_i(y) \, dA$$

with $b_1(y) = y_1^4$, $b_2(y) = y_2^4$, $b_3(y) = y_3^4$, $b_4(y) = y_1^3y_2$, $b_5(y) = y_1^3y_3$, $b_6(y) = y_1y_2^3$, $b_7(y) = y_2^3y_3$, $b_8(y) = y_1y_3^3$, $b_9(y) = y_2y_3^3$, $b_{10}(y) = y_1^2y_2^2$, $b_{11}(y) = y_1^2y_3^2$, $b_{12}(y) = y_2^2y_3^2$, $b_{13}(y) = y_1^2y_2y_3$, $b_{14}(y) = y_1y_2^2y_3$ and $b_{15}(y) = y_1y_2y_3^2$. By symmetry, we see that $B_i = 0$ for i = 4, ..., 9 and i = 13, 14, 15, These show that M_s is a linear function of the diagonal and sub-diagonal elements of \hat{W} .

Let *D* be changed to βD , where β is a positive number. For (16), it involves an integral over S_E , we may use the parametric expression

$$y = \begin{pmatrix} \frac{1}{\sqrt{\alpha_1}} \cos\theta \sin\phi \\ \frac{1}{\sqrt{\alpha_2}} \sin\theta \sin\phi \\ \frac{1}{\sqrt{\alpha_3}} \cos\phi \end{pmatrix}$$

for S_E , where $0 \leq \theta < 2\pi$, $0 \leq \phi \leq \pi$. Then

$$\iint_{S_E} f(y) dA = \int_0^{2\pi} \int_0^{\pi} f\left(\frac{1}{\sqrt{\alpha_1}}\cos\theta\sin\phi, \frac{1}{\sqrt{\alpha_2}}\sin\theta\sin\phi, \frac{1}{\sqrt{\alpha_3}}\cos\phi\right)\sin\phi$$
$$\times \sqrt{\frac{1}{\alpha_1\alpha_2}\cos^2\phi + \frac{1}{\alpha_3}\left(\frac{1}{\alpha_1}\sin^2\theta + \frac{1}{\alpha_2}\cos^2\theta\right)\sin^2\phi} \, d\phi \, d\theta,$$

where

$$f(y) = \sum_{i,j,k,l=1}^{3} \hat{W}_{ijkl} y_i y_j y_k y_l.$$

When *D* is changed to βD , α_1 , α_2 and α_3 are changed to $\beta \alpha_1$, $\beta \alpha_2$ and $\beta \alpha_3$ respectively. So this integral is multiplied with a factor $\frac{1}{\beta^3}$. For M_E in (16), this integral needs to be multiplied with $\frac{M_D^2}{S_E}$. Since M_D^2 will be changed to $\beta^2 M_D^2$ and S_E will be changed to $\frac{S_E}{\beta}$, M_E is not changed. The theorem is proved. \Box

The coefficients B_i as well as the area S_E cannot be computed exactly in general. But they also can be computed numerically. For the integral over S_E , we may use the formulas used in the proof of Theorem 5. The fundamental difference between the formulas of A_i in the last section and the formulas of B_i in this section is that A_i can be calculated in any Cartesian coordinate system while B_i only can be calculated in the inherent coordinate system. We regard M_E also as an inherent parameter. As we said in the introduction, it is a kind of weighted average AKC values.

5. The scaled inherent coordinate system

Let $z_i = \sqrt{\alpha_i} y_i$ for i = 1, 2, 3. Then the ellipsoidal surface S_E is scaled to a spherical surface

 $S_Z = \{ z \in \mathfrak{R}^3 : \ z_1^2 + z_2^2 + z_3^2 = 1 \}.$

Correspondingly, we may scale \hat{W} by

$$\bar{W}_{ijkl} = \frac{M_D^2 \hat{W}_{ijkl}}{\sqrt{\alpha_i \alpha_j \alpha_k \alpha_l}}.$$

By (5), the AKC value along the direction y is now

$$K_{\rm app} = \frac{M_D^2 \sum_{i, j,k,l=1}^3 \hat{W}_{ijkl} y_i y_j y_k y_l}{\left(\sum_{i,j=1}^3 \hat{D}_{ij} y_i y_j\right)^2} = \frac{\sum_{i,j,k,l=1}^3 \bar{W}_{ijkl} z_i z_j z_k z_l}{(z_1^2 + z_2^2 + z_3^2)^2}.$$
(18)

Then the average AKC value on the surface S_Z is

$$M_Z = \frac{1}{4\pi} \iint_{S_Z} \sum_{i,j,k,l=1}^3 \bar{W}_{ijkl} z_i z_j z_k z_l dA.$$

We now show that M_Z has a simple form. Note that $\bar{W}_{1122} + \bar{W}_{1133} + \bar{W}_{2233}$ is equal to one sixth of the sum of the sub-diagonal elements of \bar{W} .

Theorem 6. The quantity M_Z is equal to one fifth of the sum of the diagonal elements plus two fifths of the sum of the sub-diagonal elements of \overline{W} , i.e.,

$$\begin{split} M_Z &= \frac{1}{5} (\bar{W}_{1111} + \bar{W}_{2222} + \bar{W}_{3333} + 2\bar{W}_{1122} + 2\bar{W}_{1133} + 2\bar{W}_{2233}) \\ &= \frac{M_D^2}{5} \bigg(\frac{\hat{W}_{1111}}{\alpha_1^2} + \frac{\hat{W}_{2222}}{\alpha_2^2} + \frac{\hat{W}_{3333}}{\alpha_3^2} + \frac{2\hat{W}_{1122}}{\alpha_1\alpha_2} + \frac{2\hat{W}_{1133}}{\alpha_1\alpha_3} + \frac{2\hat{W}_{2233}}{\alpha_2\alpha_3} \bigg). \end{split}$$

Proof. As the proofs of Theorems 3 and 5, we may show that

$$M_Z = \frac{1}{4\pi} [C_1 \bar{W}_{1111} + C_2 \bar{W}_{2222} + C_3 \bar{W}_{3333} + 6C_{10} \bar{W}_{1122} + 6C_{11} \bar{W}_{1133} + 6C_{12} \bar{W}_{2233}],$$

where

$$C_i = \iint_{S_Z} c_i(z) \, dA$$

with $c_1(z) = z_1^4$, $c_2(z) = z_2^4$, $c_3(z) = z_3^4$, $c_{10}(z) = z_1^2 z_2^2$, $c_{11}(z) = z_1^2 z_3^2$ and $c_{12}(z) = z_2^2 z_3^2$. By symmetry, we see that $C_1 = C_2 = C_3$ and $C_{10} = C_{11} = C_{12}$. With the formula at the end of Section 3, we have

$$C_3 = \int_{0}^{2\pi} \int_{0}^{\pi} (\cos \phi)^4 \sin \phi \, d\phi \, d\theta = \frac{4\pi}{5}.$$

We also see that

$$C_1 + C_2 + C_3 + 2C_{10} + 2C_{11} + 2C_{12} = \iint_{S_Z} \left(z_1^2 + z_2^2 + z_3^2 \right)^2 dA = S_Z = 4\pi$$

Putting these together, we have the conclusion. \Box

The quantity M_Z is also an inherent parameter and a kind of weighted average AKC values. But its computational formula is much simpler.

We now show that M_Z is equal to one fifth of the sum of the six Kelvin eigenvalues of \overline{W} .

Theorem 7. The quantity M_Z is equal to one fifth of the sum of the six Kelvin eigenvalues of \overline{W} .

Proof. By the discussion in Section 2, we know that the six Kelvin eigenvalues of \overline{W} are the six eigenvalues of the following matrix \overline{U} :

$$\bar{U} = \begin{pmatrix} \bar{W}_{1111} & \bar{W}_{1122} & \bar{W}_{1133} & \sqrt{2}\bar{W}_{1112} & \sqrt{2}\bar{W}_{1113} & \sqrt{2}\bar{W}_{1123} \\ \bar{W}_{1122} & \bar{W}_{2222} & \bar{W}_{2233} & \sqrt{2}\bar{W}_{1222} & \sqrt{2}\bar{W}_{1223} & \sqrt{2}\bar{W}_{2223} \\ \bar{W}_{1133} & \bar{W}_{2233} & \bar{W}_{3333} & \sqrt{2}\bar{W}_{1233} & \sqrt{2}\bar{W}_{1333} & \sqrt{2}\bar{W}_{2333} \\ \sqrt{2}\bar{W}_{1112} & \sqrt{2}\bar{W}_{1222} & \sqrt{2}\bar{W}_{1233} & 2\bar{W}_{1122} & 2\bar{W}_{1123} & 2\bar{W}_{1223} \\ \sqrt{2}\bar{W}_{1113} & \sqrt{2}\bar{W}_{1223} & \sqrt{2}\bar{W}_{1333} & 2\bar{W}_{1123} & 2\bar{W}_{1233} \\ \sqrt{2}\bar{W}_{1123} & \sqrt{2}\bar{W}_{2223} & \sqrt{2}\bar{W}_{2333} & 2\bar{W}_{1223} & 2\bar{W}_{1233} & 2\bar{W}_{2233} \end{pmatrix}.$$

Since the sum of the six eigenvalues of \overline{U} is the sum of the diagonal elements of \overline{U} (the trace of \overline{U}), by Theorem 6, the conclusion of this theorem holds. \Box

This theorem shows that after adequate scaling (this scaling corresponds to adding the *D* coefficients in the constraints of (7) and (8) to (12) and (13), the average Kelvin eigenvalues is corresponding to the average AKC value on a certain surface. The following is some further relationship between the AKC values and the Kelvin eigenvalues of \overline{W} .

Theorem 8. Denote the largest and the smallest Kelvin eigenvalues of \overline{W} by μ_{max} and μ_{min} . Then we have

$$\mu_{\min} \leqslant K_{\min} \leqslant K_{\max} \leqslant \mu_{\max}$$
.

(19)

The inequalities in (19) can be strict. In fact, for any number $c < \frac{4}{3}$, there is an example such that $\mu_{max} \ge cK_{max}$.

Proof. For any two second order three-dimensional tensors $X = (X_{ij})$ and $Y = (Y_{ij})$, denote their inner product as

$$X^T Y = \sum_{i,j=1}^3 X_{ij} Y_{ij}$$

Let *y* be a direction. By (18), there is a $z \in S_E$ such that the AKC value at the direction *y* is

$$K_{\text{app}} = \sum_{i,j,k,l=1}^{3} \bar{W}_{ijkl} z_i z_j z_k z_l = X^T \bar{W} X = v^T \bar{U} v,$$

where $X = (z_i z_j)$ and $v = (z_1^2, z_2^2, z_3^2, \sqrt{2}z_1 z_2, \sqrt{2}z_1 z_3, \sqrt{2}z_2 z_3)^T$. Then

$$v^T v = (z_1^2 + z_2^2 + z_3^2)^2 = 1.$$

By linear algebra, we have

$$\mu_{\min} \leq v^T U v \leq \mu_{\max}.$$

This proves (19). Now let $\bar{W}_{iiii} = 1$ for i = 1, 2, 3, and other \bar{W}_{ijkl} are zero. We see that $K_{\min} = \frac{1}{3}$ in this example but $\mu_{\min} = 0$. This shows that the first equality in (19) can be strict. Let $\bar{W}_{iiii} = 1$ for i = 1, 2, 3, $\bar{W}_{1122} = \bar{W}_{1212} = \bar{W}_{1212} = \bar{W}_{2112} = a > 1$ and other \bar{W}_{ijkl} are zero. Then $K_{\min} = \frac{1}{2}$, $K_{\max} = \frac{1+3a}{2}$, and $\mu_{\max} = 2a$. This proves the remaining conclusions. \Box

The first conclusion of this theorem shows that after adequate scaling, the largest Kelvin eigenvalue is an upper bound of the AKC value, while the smallest Kelvin eigenvalue is a lower bound of the AKC value. The second conclusion of this theorem shows it is possible that such an upper bound is greater than the largest AKC value and such a lower bound is smaller than the smallest AKC value. On the other hand, Theorem 1 indicates that the largest and the smallest D-eigenvalues, after multiplied by M_D^2 , equal to the largest and the smallest AKC values. These further show that D-eigenvalues are better tools to study the extremal AKC values.

6. Numerical examples

In this section, we report some computational results on the principal invariants and inherent parameters of some diffusion kurtosis tensors derived from data of MRI experiments on rat spinal cord specimen fixed in formalin. The MRI experiments were conducted on a 7 Tesla MRI scanner at Laboratory of Biomedical Imaging and Signal Processing at The University of Hong Kong.

In MRI experiments, the AKC and ADC values for a given gradient $x \in \Re^3$ can be determined by acquiring data at three or more *b* values [8] including b = 0. In our experiments, we take six *b* values 0, 800, 1600, 2400, 3200 and 4000, in unit of s/mm². In each example, we take 30 gradient directions and get the corresponding AKC and ADC values as the averages of

	<i>x</i> ₁	<i>x</i> ₂	<i>x</i> ₃	$\lambda imes 10^{-7}$	AKC
1	-26.6953	-76.0271	13.2301	3.8340	2.1782
2	8.3561	-69.1354	28.6108	2.4323	1.3819
3	58.9844	-42.6590	17.9274	0.6773	0.3848
4	-62.4736	-35.3967	20.0392	3.8173	2.1687
5	29.1437	-52.2572	33.9600	2.4900	1.4146
6	34.8925	49.2278	31.7172	1.0247	0.5822
7	-21.9794	-31.4925	44.7823	-0.0738	-0.0419
8	24.4491	-12.3897	46.0146	2.0092	1.1415
9	-12.2897	23.6850	47.6412	2.0563	1.1682
10	-66.1780	11.3946	25.5877	5.3545	3.0420
11	11.5202	18.0765	47.7258	2.2194	1.2609
12	65.6942	7.1795	21.9765	-1.2420	-0.7056

Table 1D-eigenvalues and eigenvectors of W

the 100 pixels. From these ADC and AKC values, we obtain the elements of the diffusion tensor D and the diffusion kurtosis tensor W by the using the least squares method and (6), as suggested in [8] and [11].

Our first example is taken from the white matter. The diffusion tensor D is

$$D = \begin{pmatrix} 0.1755 & 0.0035 & 0.0132 \\ 0.0035 & 0.1390 & 0.0017 \\ 0.0132 & 0.0017 & 0.4006 \end{pmatrix} \times 10^{-3}$$

in unit of square mm per second, and the fifteen independent elements of the diffusion kurtosis tensor W are $W_{1111} = 0.4982$, $W_{2222} = 0$, $W_{3333} = 2.6311$, $W_{1112} = -0.0582$, $W_{1113} = -1.1719$, $W_{1222} = 0.4880$, $W_{2223} = -0.6162$, $W_{1333} = 0.7639$, $W_{2333} = 0.7631$, $W_{1122} = 0.2236$, $W_{1133} = 0.4597$, $W_{2233} = 0.1519$, $W_{1123} = -0.0171$, $W_{1223} = 0.1852$ and $W_{1233} = -0.4087$, respectively. It is easy to find that

$$M_D^2 = \left(\frac{D_{11} + D_{22} + D_{33}}{3}\right)^2 = 5.6813 \times 10^{-8}$$

To find the largest and the smallest AKC values, we need first obtain the largest and the smallest D-eigenvalues. Using the method provided in [20], we compute all the D-eigenvalues of W, and the associated eigenvectors, which are listed in Table 1.

From the above table we can see that the largest and the smallest AKC values for this example as 3.0420 and -0.7056, attained at

$$(-66.1780, 11.3946, 25.5877)^{+}$$
 and $(65.6942, 7.1795, 21.9765)^{+}$,

respectively. The spherical average AKC value M_5 is 1.4601, which is in the interval $[K_{\min}, K_{\max}] = [-0.7056, 3.0420]$ and the six coefficients $A_1, A_2, A_3, A_{10}, A_{11}, A_{12}$ in the proof of Theorem 3 are

 $[0.2514, 0.6445, 0.8619, 0.1406, 0.1523, 0.2499] \times 10^{-8}.$

To compute the inherent parameters, we first find the eigen-decomposition of the diffusion tensor D, $\hat{D} = P^T D P$, where \hat{D} is a diagonal matrix whose diagonal elements $(\alpha_1, \alpha_2, \alpha_3) = (0.4013, 0.1751, 0.1387) * 10^{-3}$ and

$$P = \begin{pmatrix} 0.0584 & 0.9939 & 0.0938 \\ 0.0073 & 0.0935 & -0.9956 \\ 0.9983 & -0.0589 & 0.0018 \end{pmatrix}.$$

The differences among the values $(\alpha_1, \alpha_2, \alpha_3)$ are relatively large, reflecting the anisotropic property of the white matter. The fifteen independent elements of \hat{W} are $\hat{W}_{1111} = 2.8190$, $\hat{W}_{2222} = 0.7561$, $\hat{W}_{3333} = -0.1641$, $\hat{W}_{1112} = 0.7160$, $\hat{W}_{1113} = -0.6065$, $\hat{W}_{1222} = -1.1675$, $\hat{W}_{2223} = 0.0512$, $\hat{W}_{1333} = 0.6359$, $\hat{W}_{2333} = -0.4408$, $\hat{W}_{1122} = 0.1521$, $\hat{W}_{1133} = 0.2403$, $\hat{W}_{2233} = 0.3019$, $\hat{W}_{1123} = 0.4521$, $\hat{W}_{1223} = -0.1710$ and $\hat{W}_{1233} = 0.1219$, respectively. The AKC values along the three eigenvectors of D (columns of P) are respectively 0.9943, 1.4017 and -0.4848. The ellipsoidal average AKC value $M_E = 0.9812$ which is also in the interval $[K_{\min}, K_{\max}] = [-0.7056, 3.0420]$, the six coefficients $B_1, B_2, B_3, B_{10}, B_{11}, B_{12}$ in the proof of Theorem 5 are

 $[0.0450, 0.3603, 1.5698, 0.0020, 0.0757, 0.1534] \times 10^{-3},$

and $S_E = 0.3072$.

We also compute the D-eigenvalues of \hat{D} and \hat{W} and the results are the same as those listed in Table 1, showing the rotation invariant property of D-eigenvalues, as indicated by Theorem 2.

Now we check the result in Theorem 6. We compute the tensor \bar{W} by $\bar{W}_{ijkl} = \frac{M_D^2 \hat{W}_{ijkl}}{\sqrt{\alpha_i \alpha_j \alpha_k \alpha_l}}$. Then the fifteen independent elements of \bar{W} are $\bar{W}_{1111} = 0.9943$, $\bar{W}_{2222} = 1.4017$, $\bar{W}_{3333} = -0.4848$, $\bar{W}_{1112} = 0.3824$, $\bar{W}_{1113} = -0.3639$, $\bar{W}_{1222} = -1.4294$,

 $\bar{W}_{2223} = 0.1067, \ \bar{W}_{1333} = 1.1044, \ \bar{W}_{2333} = -1.1594, \ \bar{W}_{1122} = 0.1230, \ \bar{W}_{1133} = 0.2453, \ \bar{W}_{2233} = 0.7066, \ \bar{W}_{1123} = 0.4108, \ \bar{W}_{1223} = -0.2352 \text{ and } \ \bar{W}_{1233} = 0.1884, \text{ respectively.}$

We have $M_Z = 0.8122$, and the six coefficients $C_1, C_2, C_3, C_{10}, C_{11}, C_{12}$ in the proof of Theorem 6 are

[2.5133, 2.5133, 2.5133, 0.8378, 0.8378, 0.8378].

From the above number, it easy to see that the equalities in Theorem 6 hold, i.e.,

$$M_{Z} = \frac{1}{5} (\bar{W}_{1111} + \bar{W}_{2222} + \bar{W}_{3333} + 2\bar{W}_{1122} + 2\bar{W}_{1133} + 2\bar{W}_{2233})$$
$$= \frac{M_{D}^{2}}{5} \left(\frac{\hat{W}_{1111}}{\alpha_{1}^{2}} + \frac{\hat{W}_{2222}}{\alpha_{2}^{2}} + \frac{\hat{W}_{3333}}{\alpha_{3}^{2}} + \frac{2\hat{W}_{1122}}{\alpha_{1}\alpha_{2}} + \frac{2\hat{W}_{1133}}{\alpha_{1}\alpha_{3}} + \frac{2\hat{W}_{2233}}{\alpha_{2}\alpha_{3}} \right).$$

The six-dimensional matrix \overline{U} is

(0.994	3 0.	1230	0.2453	0.5408 -	-0.5147	0.5810	
0.123	0 1.	4017	0.7066 -	-2.0215 -	-0.3327	0.1509	
0.245	i3 0.	7066 -	-0.4848	0.2664	1.5619 -	-1.6396	
0.540	08 —2	2.0215	0.2664	0.2460	0.8216 -	-0.4705	•
-0.51	47 —0	.3327	1.5619	0.8216	0.4906	0.3767	
0.581	0 0.	1509 -	-1.6396 -	-0.4705	0.3767	1.4132	

The six eigenvalues of \overline{U} are 3.2568, 2.5848, -2.5724, -1.6020, 1.2318, and 1.1621, and its smallest and largest eigenvalues are -2.5724 and 3.2568 respectively. We can see that these two values are out of the range of the AKC values: [-0.7056, 3.0420].

Our second example is taken from the gray matter. The diffusion tensor D is

 $D = \begin{pmatrix} 0.3755 & 0.0105 & 0.0013 \\ 0.0105 & 0.2603 & -0.0077 \\ 0.0013 & -0.0077 & 0.4081 \end{pmatrix} \times 10^{-3}$

in unit of square mm per second, and the fifteen independent elements of the diffusion kurtosis tensor *W* are $W_{1111} = 1.5248$, $W_{2222} = 0$, $W_{3333} = 1.9725$, $W_{1112} = 0.1276$, $W_{1113} = -0.1082$, $W_{1222} = 0.0803$, $W_{2223} = -0.1722$, $W_{1333} = 0.1994$, $W_{2333} = 0.1057$, $W_{1122} = 0.3324$, $W_{1133} = 0.2443$, $W_{2233} = 0.1581$, $W_{1123} = 0.0008$, $W_{1223} = -0.0526$ and $W_{1233} = -0.0326$, respectively. The largest and the smallest AKC values for this example are 1.5022 and -0.1587, attained at (6.8833, 6.3098, 48.8746)^T and (-2.3765, 60.2395, 12.9539)^T, respectively. The spherical average AKC value M_S is 1.1068. To compute the inherent parameters, we first find the eigen-decomposition of the diffusion tensor D, $\hat{D} = P^T DP$, where \hat{D} is a diagonal matrix whose diagonal elements ($\alpha_1, \alpha_2, \alpha_3$) = (0.4085, 0.3764, 0.2589) and

 $P = \begin{pmatrix} 0.0246 & 0.9956 & -0.0899 \\ -0.0500 & 0.0911 & 0.9946 \\ 0.9984 & -0.0200 & 0.0520 \end{pmatrix}.$

The differences among the values $(\alpha_1, \alpha_2, \alpha_3)$ are relatively small, reflecting the isotropic property of the grey matter. The fifteen independent elements of \hat{W} are $\hat{W}_{1111} = 1.9625$, $\hat{W}_{2222} = 1.5702$, $\hat{W}_{3333} = -0.0423$, $\hat{W}_{1112} = 0.1877$, $\hat{W}_{1113} = 0.1601$, $\hat{W}_{1222} = -0.0944$, $\hat{W}_{2223} = 0.0712$, $\hat{W}_{1333} = -0.1270$, $\hat{W}_{2333} = -0.0171$, $\hat{W}_{1122} = 0.2258$, $\hat{W}_{1133} = 0.1896$, $\hat{W}_{2233} = 0.3228$, $\hat{W}_{1123} = -0.0250$, $\hat{W}_{1223} = -0.0023$ and $\hat{W}_{1233} = -0.0674$, respectively. The AKC values along the three eigenvectors of *D* are respectively 1.4239, 1.3416 and -0.0764. The ellipsoidal average AKC value $M_E = 1.2351$.

Now we check the result in Theorem 6. We compute the tensor \bar{W} by $\bar{W}_{ijkl} = \frac{M_D^2 \hat{W}_{ijkl}}{\sqrt{\alpha_i \alpha_j \alpha_k \alpha_l}}$. The fifteen independent elements of \bar{W} are $\bar{W}_{1111} = 1.4239$, $\bar{W}_{2222} = 1.3416$, $\bar{W}_{3333} = -0.0764$, $\bar{W}_{1112} = 0.1419$, $\bar{W}_{1113} = 0.1459$, $\bar{W}_{1222} = -0.0775$, $\bar{W}_{2223} = 0.0734$, $\bar{W}_{1333} = -0.1826$, $\bar{W}_{2333} = -0.0257$, $\bar{W}_{1122} = 0.1778$, $\bar{W}_{1133} = 0.2170$, $\bar{W}_{2233} = 0.4010$, $\bar{W}_{1123} = -0.0238$, $\bar{W}_{1223} = -0.0022$ and $\bar{W}_{1233} = -0.0803$, respectively.

We have $M_Z = 0.8561$. The six-dimensional matrix \overline{U} is

(1.4239	0.1778	0.2170	0.2007	0.2064	-0.0336
0.1778	1.3416	0.4010	-0.1096	-0.0031	0.1038
0.2170	0.4010	-0.0764	-0.1136	-0.2583	-0.0363
0.2007	-0.1096	-0.1136	0.3556	-0.0475	-0.0045
0.2064	-0.0031	-0.2583	-0.0475	0.4340	-0.1607
-0.0336	0.1038	-0.0363	-0.0045	-0.1607	0.8020

whose six eigenvalues are 1.6778, 1.3338, 0.8244, 0.4686, -0.3347, 0.3107. Its smallest and largest eigenvalues are -0.3347 and 1.6778 respectively. Again, they are out of the AKC value range: [-0.1587, 1.5022].



Fig. 1. The map of M_S .



Fig. 2. The map of M_E .

Figs. 1–5 show the maps of M_S , M_E , M_Z , the largest and the smallest AKC values, respectively, on the rat spinal cord samples. In the figures, the values are scaled to [0, 1], where 0 is the darkest part, and 1 is the brightest part. The ranges of M_S , M_E , M_Z , the largest and the smallest AKC values are M_S : [-0.1285, 0.5191]; M_E : [-0.2761, 0.8099]; M_Z : [-1.8371, 2.0628]; K_{max} : [0.0001, 6.9012]; and K_{min} : [-3.2542, 0.5852] respectively.

7. Final remarks

In this paper, we studied some principal invariants and inherent parameters of a DK tensor W. The largest AKC value K_{max} , the smallest AKC value K_{min} and the spherical average AKC value M_S are the principal invariants of W. They can be calculated in any Cartesian coordinate system. The inherent form \hat{W} and its elements, the ellipsoidal average AKC value M_E , and the weighted average AKC value M_Z are inherent parameters. They must be calculated in the inherent coordinate system of W. We hope that some of these quantities can be useful in the DKI practice.

In Sections 2 and 5, we compared the D-eigenvalues and the Kelvin eigenvalues. It is shown that the D-eigenvalues reflect exactly the largest and the smallest AKC values (Theorem 1), while the Kelvin eigenvalues, after adequate scaling, only give upper and lower bounds of AKC values, and such bounds have positive gaps with the largest and the smallest AKC values. This is not surprising in mathematics, as the Kelvin eigenvalue approach regards the vector product (x_ix_j) as a matrix $X = (X_{ij})$, then drops the rank-one restriction on X. The Kelvin eigenvector X in general is not a rank-one matrix,



Fig. 3. The map of M_Z .



Fig. 4. The map of the largest AKC.

i.e., we cannot make $X_{ij} = x_i x_j$ in general. Thus, the Kelvin approach inevitably produces positive gaps when they are used to estimate the largest and the smallest AKC values. On the other hand, the D-eigenvalue approach generates the largest and the smallest AKC values exactly, as Theorem 1 indicates. Besides, Theorem 6 indicates that the sum of the Kelvin eigenvalues is related with M_Z . This shows that Kelvin eigenvalues are closer to the average AKC values in a certain sense.

Actually, a fourth order tensor W is a multi-linear operator

$$g(x, y, z, w) = \sum_{i, j, k, l=1}^{3} W_{ijkl} x_i y_j z_k w_l.$$

The Kelvin eigenvalue approach treats W as a linear operator

$$g(X,Y) = \sum_{i,j,k,l=1}^{3} W_{ijkl} X_{ij} Y_{kl}.$$

This certainly misses the multi-linearity information of *W*.

In Section 6, we presented two numerical examples based upon the MRI data acquired out of rat spinal cord samples. In these two examples, W has 12 D-eigenvalues. This reflects that the optimization problems (7) and (8) are highly nonlinear,



Fig. 5. The map of the smallest AKC.

namely, with a quartic objective function and a quadratic constraint, which result in possibly 12 critical points. Among these 12 D-eigenvalues, the largest and the smallest one are more meaningful. They reflect the largest and the smallest AKC values. The other D-eigenvalues are local maximum, local minimum and saddle point AKC values. They are less important.

In these two examples, some AKC values are negative. A negative AKC value means that the diffusion displacement probability distribution is more sharply peaked than a Gaussian distribution; while a positive AKC values implies the diffusion displacement probability distribution is less sharply peaked than a Gaussian distribution. To ensure the model has physical meaning, we only need to guarantee that

$$bD_{\rm app} - \frac{1}{6}b^2 D_{\rm app}^2 K_{\rm app} \tag{20}$$

is positive along any direction. To guarantee the positivity of the above function, it suffices that the diffusion tensor *D* is positive definite and the *b*-value chosen to fit Eq. (4) is smaller than $b_{\min} := 3/(D_{app}K_{app})$. How can we guarantee a positive definite diffusion tensor *D*? This problem has only been recently tackled in the literature related to Diffusion Tensor Imaging. See for example [4,23]. How to obtain a positive definite diffusion tensor *D* and to guarantee the positiveness of (20) should be further studied carefully.

Recently, there are increasing interests on invariants of a fourth order tensor, such as the elasticity tensor in solid mechanics [12,13].

In this paper, we mainly study invariants of the DK tensor *W* from the mathematical side. A further collaboration of applied mathematicians and biomedical engineering researchers may further reveal the physical, biological and clinical meanings of such invariants.

Appendix A. Calculation of D-eigenvalues and D-eigenvectors

From the definition of the D-eigenvalues and D-eigenvectors (9), for finding these values, we need to solve the polynomial equations (9). A direct method for solving such polynomial equations was introduced in [20]. Here we describe that method to make our paper self-contained.

Let W be the fourth-order symmetric tensor, whose elements are defined as

$$\tilde{W}_{ijkl} = \sum_{i'=1}^{3} D_{ii'}^{-1} W_{i'jkl}, \quad i, j, k, l = 1, 2, 3.$$

Then, (9) can be reformulated as

2

4

$$\begin{cases} \sum_{j,k,l=1}^{3} \tilde{W}_{ijkl} x_j x_k x_l = \lambda x_i, & i = 1, 2, 3, \\ \sum_{i,j=1}^{3} D_{ij} x_i x_j = 1. \end{cases}$$
(A.1)

We have the following result, which is Theorem 4 in [20]. The proof is omitted here and the interested reader is referred to [20].

Theorem A.1.

(a) If $\tilde{W}_{2111} = \tilde{W}_{3111} = 0$, then $\lambda = \frac{\tilde{W}_{1111}}{D_{11}}$ is a D-eigenvalue with a D-eigenvector $x = (\pm \sqrt{\frac{1}{D_{11}}}, 0, 0)^{\top}$. (b) For any real root t of the following equations

$$\begin{cases} -\tilde{W}_{2111}t^4 + (\tilde{W}_{1111} - 3\tilde{W}_{2112})t^3 + 3(\tilde{W}_{1112} - \tilde{W}_{2122})t^2 + (3\tilde{W}_{1122} - \tilde{W}_{2222})t + \tilde{W}_{1222} = 0, \\ \tilde{W}_{3111}t^3 + 3\tilde{W}_{3112}t^2 + 3\tilde{W}_{3122}t + \tilde{W}_{3222} = 0, \\ x = \pm \frac{1}{\sqrt{D_{11}t^2 + 2D_{12}t + D_{22}}} (t, 1, 0)^\top$$
(A.2)

is a D-eigenvector of W with the D-eigenvalue $\lambda = \sum_{i,j,k,l=1}^{3} W_{ijkl} x_i x_j x_k x_l$. (c) For any real root u and v of the following solutions

$$\begin{cases} -\tilde{W}_{3111}u^4 - 3\tilde{W}_{3112}u^3v + (\tilde{W}_{1111} - 3\tilde{W}_{3113})u^3 - 3\tilde{W}_{3122}u^2v^2 + (3\tilde{W}_{1112} - 6\tilde{W}_{3123})u^2v \\ + (3\tilde{W}_{1113} - 3W_{3133})u^2 - 3W_{3223}uv^2 - \tilde{W}_{3222}uv^3 + 3\tilde{W}_{1122}uv^2 + (6\tilde{W}_{1123} - 3\tilde{W}_{3233})uv \\ + (3\tilde{W}_{1133} - \tilde{W}_{3333})u + \tilde{W}_{1222}v^3 + 3\tilde{W}_{1223}v^2 + 3\tilde{W}_{1233}v + \tilde{W}_{1333} = 0, \\ -\tilde{W}_{3111}u^3v + \tilde{W}_{2111}u^3 - 3\tilde{W}_{3112}u^2v^2 + (3\tilde{W}_{2112} - 3\tilde{W}_{3113})u^2v + 3\tilde{W}_{2113}u^2 - 3\tilde{W}_{3122}uv^3 \\ + (3\tilde{W}_{2122} - 6\tilde{W}_{3123})uv^2 + (6\tilde{W}_{2123} - 3\tilde{W}_{3133})uv + 3\tilde{W}_{2133}u + 3\tilde{W}_{2223}v^2 - \tilde{W}_{3222}v^4 \\ + (\tilde{W}_{2222} - 3\tilde{W}_{3223})v^3 - 3\tilde{W}_{3233}v^2 + (3\tilde{W}_{2233} - \tilde{W}_{3333})v + \tilde{W}_{2333} = 0, \\ x = \pm \frac{1}{\sqrt{D_{11}u^2 + 2D_{12}uv + D_{22}v^2 + 2D_{23}v + D_{33}}} (u, v, 0)^{\top}$$
(A.3)

is a D-eigenvector of W with the D-eigenvalue $\lambda = \sum_{i,j,k,l=1}^{3} W_{ijkl} x_i x_j x_k x_l$.

All the D-eigenpairs of tensors D and W are given by (a)–(c) if $\tilde{W}_{2111} = \tilde{W}_{3111} = 0$, and by (b) and (c) otherwise.

From the above theorem, we can see that the main task in finding the D-eigenvalues and D-eigenvectors is to solve the systems (A.2) and (A.3). (A.2) is a system of polynomial equations with a single variable t, which can be solved easily. (A.3) is a system of polynomial equations in two variables u and v. For solving such a system, we first regard it as a system of polynomial equations of variable u and rewrite it as

$$\begin{cases} \gamma_0 u^4 + \gamma_1 u^3 + \gamma_2 u^2 + \gamma_3 u + \gamma_4 = 0, \\ \tau_0 u^3 + \tau_1 u^2 + \tau_2 u + \tau_3 = 0, \end{cases}$$

where $\gamma_0, \ldots, \gamma_4, \tau_0, \ldots, \tau_3$ are polynomials of v, which can be calculated by (A.3). The above system of polynomial equations in u possesses solutions if and only if its resultant vanishes [5]. The resultant of this system of polynomial equations is the determinant of the following 7×7 matrix

	(γ0	γ_1	γ_2	γ_3	γ_4	0	0 /	
	0	γ_0	γ_1	γ_2	γ3	γ_4	0	
	0	0	γ_0	γ_1	γ_2	γ3	γ_4	
V :=	$ au_0$	$ au_1$	$ au_2$	$ au_3$	0	0	0	,
	0	$ au_0$	$ au_1$	$ au_2$	$ au_3$	0	0	
	0	0	$ au_0$	$ au_1$	$ au_2$	$ au_3$	0	
	0/	0	0	τ_0	τ_1	τ2	τ_3	

which is a polynomial equation in variable v. After finding all real roots of this polynomial, we can substitute them to (A.3) to find all the real solutions of u. Correspondingly, all the D-eigenvalues and the corresponding D-eigenvectors can be found.

References

- A. Barmpoutis, B. Jian, B.C. Vemuri, T.M. Shepherd, Symmetric positive 4th order tensors and their estimation from diffusion weighted MRI, in: M. Karssemeijer, B. Lelieveldt (Eds.), Information Processing and Medical Imaging, Springer-Verlag, Berlin, 2007, pp. 308–319.
- [2] PJ. Basser, D.K. Jones, Diffusion-tensor MRI: Theory, experimental design and data analysis—a technical review, Nucl. Magn. Reson. Biomed. 15 (2002) 456–467.
- [3] PJ. Basser, S. Pajevic, Spectral decomposition of a 4th-order covariance tensor: Applications to diffusion tensor MRI, Signal Process. 87 (2007) 220-236.
- [4] C. Chefd'Hotel, D. Tschumperle, R. Deriche, O. Faugeras, Regularizing flows for constrained matrix-valued images, J. Math. Imaging Vision 20 (2004) 147–162.

- [5] D. Cox, J. Little, D. O'Shea, Using Algebraic Geometry, Springer-Verlag, New York, 1998.
- [6] P.K. Ghosh, D.S. Jayas, E.A. Smith, M.L.H. Gruwel, N.D.G. White, Mathematical modelling of wheat kernel drying with input from moisture movement studies using magnetic resonance imaging (MRI), Part II: Model comparison with published studies, Biosyst. Eng. 100 (2008) 547–554.
- [7] E.S. Hui, M.M. Cheung, L. Qi, E.X. Wu, Towards better MR characterization of neural tissues using directional diffusion kurtosis analysis, Neuroimage 42 (2008) 122–134.
- [8] J.H. Jensen, J.A. Helpern, A. Ramani, H. Lu, K. Kaczynski, Diffusional kurtosis imaging: The quantification of non-Gaussian water diffusion by means of magnetic resonance imaging, Magn. Reson. Med. 53 (2005) 1432-1440.
- [9] M. Kyriakopoulos, Th. Bargiotas, G.J. Barker, S. Frangou, Diffusion tensor imaging in schizophrenia, Eur. Psychiatry 23 (2008) 255-273.
- [10] C. Liu, R. Bammer, B. Acar, M.E. Mosely, Characterizing non-Gaussian diffusion by generalized diffusion tensors, Magn. Reson. Med. 51 (2004) 924–937.
 [11] H. Lu, J.H. Jensen, A. Ramani, J.A. Helpern, Three-dimensional characterization of non-Gaussian water diffusion in humans using diffusion kurtosis imaging, Nucl. Magn. Reson. Biomed. 19 (2006) 236–247.
- [12] M. Moakher. On the averaging of symmetric positive-definite tensors. J. Elasticity 82 (2006) 273-296.
- [13] M. Moakher, A.N. Norris, The closest elastic tensor of arbitrary symmetry to an elasticity tensor of lower symmetry, J. Elasticity 85 (2006) 215-263.
- [14] P.M. Morse, H. Feschbach, Methods of Theoretic Physics, vol. 1, McGraw-Hill, New York, 1979, p. 519.
- [15] G. Ni, L. Qi, F. Wang, Y. Wang, The degree of the E-characteristic polynomial of an even order tensor, J. Math. Anal. Appl. 329 (2007) 1218-1229.
- [16] E. Ozarslan, T.H. Mareci, Generalized diffusion tensor imaging and analytical relationships between diffusion tensor imaging and high angular resolution diffusion imaging, Magn. Reson. Med. 50 (2003) 955–965.
- [17] L. Qi, Eigenvalues of a real supersymmetric tensor, J. Symbolic Comput. 40 (2005) 1302-1324.
- [18] L. Qi, Rank and eigenvalues of a supersymmetric tensor, a multivariate homogeneous polynomial and an algebraic surface defined by them, J. Symbolic Comput. 41 (2006) 1309–1327.
- [19] L. Qi, Eigenvalues and invariants of tensors, J. Math. Anal. Appl. 325 (2007) 1363-1377.
- [20] L. Qi, Y. Wang, E.X. Wu, D-Eigenvalues of diffusion kurtosis tensors, J. Comput. Appl. Math., in press, doi:10.1016/j.cam.2007.10.012.
- [21] W. (Lord Kelvin) Thomson, Elements of a mathematical theory of elasticity, Philos. Trans. R. Soc. 166 (1856) 481.
- [22] W. (Lord Kelvin) Thomson, Elasticity, in: Encyclopedia Britannica, vol. 7, ninth ed., Adam and Charles Black, London, Edinburgh, 1878, pp. 796-825.
- [23] Z. Wang, B.C. Vemuri, Y. Chen, T.H. Mareci, A constrained variational principle for direct estimation and smoothing of the diffusion tensor field from complex DWI, IEEE Trans. Med. Imaging 23 (2004) 930–939.