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D-eigenvalues of diffusion kurtosis tensors^{*}

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Abstract

Diffusion kurtosis imaging (DKI) is a new model in medical engineering, where a diffusion kurtosis (DK) tensor is involved. A DK tensor is a fourth-order three-dimensional fully symmetric tensor. In this paper, we introduce *D*-eigenvalues for a DK tensor. The largest, the smallest and the average *D*-eigenvalues of a DK tensor correspond with the largest, the smallest and the average apparent kurtosis coefficients (AKC) of a water molecule in the space, respectively. We present their computational methods and discuss related anisotropy value of AKC.

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1. Introduction

A popular magnetic resonance imaging (MRI) model in medical engineering is called diffusion tensor imaging (DTI) [1,4]. The MR measurement of an effective diffusion tensor of water in tissues can provide unique biologically and clinically relevant information that is not available from other imaging modalities. A diffusion tensor *D* is a second-order three-dimensional fully symmetric tensor. It has six independent elements. After obtaining the values of these six independent elements by MRI techniques, the medical engineering researchers will further calculate some characteristic quantities of this diffusion tensor. These characteristic quantities are rotationally invariant, independent from the choice of the laboratory coordinate system. They include the three eigenvalues $\lambda_1 \ge \lambda_2 \ge \lambda_3$ of *D*, the mean diffusivity (M_D), the fractional anisotropy (*FA*), etc. The largest eigenvalue λ_1 describes the diffusion coefficient in the direction parallel to the fibres in the human tissue. The other two eigenvalues describe the diffusion coefficient in the direction perpendicular to the fibres in the human tissue. The mean diffusivity is

$$M_D = \frac{\lambda_1 + \lambda_2 + \lambda_3}{3},$$

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while the fractional anisotropy is

$$FA = \sqrt{\frac{3}{2}} \sqrt{\frac{(\lambda_1 - M_D)^2 + (\lambda_2 - M_D)^2 + (\lambda_3 - M_D)^2}{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}},$$

where $0 \le FA \le 1$. If FA = 0, the diffusion is isotropic. If FA = 1, the diffusion is anisotropic.

However, DTI is known to have a limited capability in resolving multiple fibre orientations within one voxel. 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 modeling of self-diffusion by a second-order tensor breaks down [5]. Recently, a new MRI model has been presented by medical engineering researchers [3,6]. They 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.

What are the coordinate system independent characteristic quantities of the DK tensor W? Are there some types of eigenvalues of W, which can play a role here? Recently, Qi introduced in [10] H-eigenvalues and Z-eigenvalues for higher-order tensors, and proved in [12] that Z-eigenvalues are invariant under coordinate system changes. Some further discussions on and applications of Z-eigenvalues can be found in [8,9,11,14]. However, physically, the concept of Z-eigenvalues cannot been applied to a DK tensor directly. In this paper, we introduce D-eigenvalues for a DK tensor W. Here, the letter "D" means diffusion. The D-eigenvalues of W are related with the diffusion tensor D. The largest, the smallest and the average D-eigenvalues of a DK tensor correspond with the largest, the smallest and the average apparent kurtosis coefficients (AKC) of a water molecule in the space, respectively. We present their computational methods and discuss the related anisotropy value of AKC.

The remaining part of this paper is distributed as follows. In Section 2, we will define these quantities and discuss their properties. We present computational methods for *D*-eigenvalues in Section 3. A numerical example is given in Section 4. Some further discussions are in Section 5.

2. Definition and properties of D-eigenvalues

We use the notation in [10–12] for the tensor and vectors. 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 [3,6]. Then the apparent diffusion coefficient (ADC) is

$$D_{\rm app} = Dx^2 \equiv \sum_{i,j=1}^3 D_{ij} x_i x_j.$$

A key formula for the DK tensor W is as follows [3,6]:

$$K_{\rm app} = \frac{M_D^2}{D_{\rm app}^2} W x^4,\tag{1}$$

where K_{app} is the apparent kurtosis coefficient in the direction x, and

$$Wx^4 \equiv \sum_{i,j,k,l=1}^3 W_{ijkl} x_i x_j x_k x_l.$$

As noted in the introduction, D and W are fully symmetric. It is known that Dx is a vector in \Re^3 with its *i*th component as

$$(Dx)_i = \sum_{j=1}^3 D_{ij} x_j,$$

for i = 1, 2, 3. As in [10–12], we denote Wx^3 as a vector in \Re^3 with its *i*th component as

$$(Wx^3)_i = \sum_{j,k,l=1}^3 W_{ijkl} x_j x_k x_l,$$

for i = 1, 2, 3. It is easy to see that maximizing (minimizing) K_{app} is equivalent to the following maximization (minimization) problem:

$$\begin{array}{l}
\max \quad Wx^4 \\
\text{s.t.} \quad Dx^2 = 1.
\end{array}$$
(2)

Without loss of generality, we may assume that D is positive definite. In practice, this assumption is natural, as ADC should be positive in general.

Obviously, the critical points of problem (2) satisfy the following equation for some $\lambda \in \mathfrak{R}$:

$$\begin{cases} Wx^3 = \lambda Dx, \\ Dx^2 = 1. \end{cases}$$
(3)

A real number λ satisfying (3) with a real vector x is called a *D***-eigenvalue** of W, and the real vector x is called a *D***-eigenvector** of W associated with the *D*-eigenvalue λ .

Theorem 1. D-eigenvalues always exist. If x is a D-eigenvector associated with a D-eigenvalue λ , then

$$\lambda = W x^4. \tag{4}$$

The largest AKC value is equal to $M_D^2 \lambda_{\text{max}}$, and the smallest AKC value is equal to $M_D^2 \lambda_{\text{min}}$, where λ_{max} and λ_{min} are the largest and the smallest D-eigenvalues of W respectively.

Proof. The feasible region of (2) is compact. The objective function of (2) is continuous. Hence, the optimization problem (2) has at least a maximizer and a minimizer. They are critical points of (2) and satisfy (3) with corresponding Lagrangian multipliers. Hence, *D*-eigenvalues always exist. By (3), we have (4). According to the optimization theory, (1) and (4), we see that the other conclusions of this theorem also hold. \Box

This theorem justifies our definition of *D*-eigenvalues.

We may use the second equation of (3) to homogenize the first equation of (3) as

$$Wx^3 = \lambda (Dx^2) Dx. \tag{5}$$

According to algebraic geometry [2], the resultant of (5) is a one-dimensional polynomial ϕ of λ . We call $\phi(\lambda)$ the *D*-characteristic polynomial of *W*.

Theorem 2. A *D*-eigenvalue is always a real root of the D-characteristic polynomial $\phi(\lambda)$.

Proof. According to the resultant theory [2], the Eq. (5) has a nonzero complex solution *x* if and only if λ is a root of its resultant. The conclusion follows.

Note that a real root of $\phi(\lambda)$ may not be a *D*-eigenvalue, as at such a real root (5) may have only conjugate complex solutions *x*. See [10] for the discussion on E-eigenvalues and *Z*-eigenvalues.

We say that W is regular if the following system has no nonzero complex solutions:

$$\begin{cases} Wx^3 = 0, \\ Dx^2 = 0. \end{cases}$$
(6)

When W is irregular, $\phi(\lambda)$ is a zero polynomial. A further study is needed in this case.

With an approach similar to that used in [8], we may conclude that the degree of ϕ is at most 13. Then, in the regular case, the number ν of *D*-eigenvalues of *W* satisfies $\nu \leq 13$. We may order the *D*-eigenvalues as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{\nu}$. Then $\lambda_1 = \lambda_{\max}$ and $\lambda_{\nu} = \lambda_{\min}$.

We define the mean kurtosis value

$$M_K = \frac{1}{\nu} \sum_{i=1}^{\nu} \lambda_i,$$

and the fractional kurtosis anisotropy as

$$FA_K = \sqrt{\frac{\nu}{\nu - 1}} \sqrt{\frac{\sum_{i=1}^{\nu} (\lambda_i - M_K)^2}{\sum_{i=1}^{\nu} \lambda_i^2}}.$$

Then we have the average AKC value as $M_D^2 M_K$, and $0 \le F A_K \le 1$. If $F A_K = 0$, the diffusion kurtosis is isotropic. If $F A_K = 1$, the diffusion kurtosis is anisotropic.

Theorem 3. D-eigenvalues, M_K and FA_K are invariant under rotations of coordinate systems.

Proof. With a rotation, x, D and W are converted to x = Py, $\hat{D} = DP^2$ and $\hat{W} = WP^4$, where $P = (p_{ij})$ is the rotation matrix, 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 [10] for the definition of orthogonal similarity. If λ is a *D*-eigenvalue with a *D*-eigenvector *x*, then by (3) and the above discussion, we have

$$\begin{cases} \hat{W}y^3 = \lambda \hat{D}y, \\ \hat{D}y^2 = 1. \end{cases}$$

This implies that *D*-eigenvalues are invariant under rotations of coordinate systems. Since M_K and FA_K are functions of *D*-eigenvalues, they are also invariant under rotations of coordinate systems.

3. Computation of *D*-eigenvalues

We cannot use the *D*-characteristic polynomial to calculate *D*-eigenvalues. First, it is difficult to calculate the resultant of a system of more than two variables [2]. Second, some real roots of the *D*-characteristic polynomial may not be *D*-eigenvalues, as stated in Section 2. It is difficult to distinguish which real roots of the *D*-characteristic polynomial are *D*-eigenvalues. Third, in the irregular case, the *D*-characteristic polynomial is a zero polynomial, which does not make any sense. Fourth, in practice, it is not enough to have *D*-eigenvalues only, but also desirable to know the *D*-eigenvectors as they are the directions at which those special AKC values apply. In this section, we present a direct method to find all the *D*-eigenvalues and their corresponding *D*-eigenvectors. The key idea here is to reduce the three variable system (3) to a system of two variables. Here, we regard λ as a parameter instead of a variable. Then, we may use the Sylvester formula of the resultant of a two variable system [2] to solve this system. As assumed in Section 2, we assume that *D* is positive definite. Then its three diagonal elements D_{11} , D_{22} and D_{33} are positive. It is also not difficult to find its inverse $D^{-1} = (\bar{d}_{ij})$. We now transform system (3) to

$$\begin{cases} D^{-1}(Wx^3) = \lambda x, \\ Dx^2 = 1. \end{cases}$$

By a short deduction, we can write the system above as

$$\begin{cases} \bar{W}x^3 = \lambda x, \\ Dx^2 = 1 \end{cases}$$
(7)

where \bar{W} is a fourth-order three-dimensional tensor such that its entries satisfy $\bar{W}_{ijkl} = \sum_{h=1}^{3} \bar{d}_{ih} W_{hjkl}$ for i, j, k, l = 1, 2, 3. Note that although the tensor \bar{W} is not fully symmetric, it is symmetric with respect to the last three indices.

Based on this conversion, we have the following theorem.

Theorem 4. (a) If $\bar{W}_{2111} = \bar{W}_{3111} = 0$, then $\lambda = \frac{\bar{W}_{1111}}{D_{11}}$ is a *D*-eigenvalue of *W* with a *D*-eigenvector $x = (\pm \sqrt{\frac{1}{D_{11}}}, 0, 0)^{\top}$.

(b) For any real root t of the following equations:

$$\begin{cases} -\bar{W}_{2111}t^4 + (\bar{W}_{1111} - 3\bar{W}_{2112})t^3 + 3(\bar{W}_{1112} - \bar{W}_{2122})t^2 + (3\bar{W}_{1122} - \bar{W}_{2222})t + \bar{W}_{1222} = 0, \\ \bar{W}_{3111}t^3 + 3\bar{W}_{3112}t^2 + 3\bar{W}_{3122}t + \bar{W}_{3222} = 0, \end{cases}$$
(8)

$$x = \pm \frac{1}{\sqrt{D_{11}t^2 + 2D_{12}t + D_{22}}} (t, 1, 0)^{\top}$$
(9)

is a D-eigenvector of W with the D-eigenvalue $\lambda = Wx^4$. (c) $\lambda = Wx^4$ and

$$x = \frac{\pm (u, v, 1)^{\top}}{D_{11}u^2 + 2D_{12}uv + 2D_{13}u + D_{22}v^2 + 2D_{23}v + D_{33}}$$
(10)

constitute a *D*-eigenpairs of *W*, where *u* and *v* are a real solution of the following polynomial equations:

$$\begin{cases} -\bar{W}_{3111}u^4 - 3\bar{W}_{3112}u^3v + (\bar{W}_{1111} - 3\bar{W}_{3113})u^3 - 3\bar{W}_{3122}u^2v^2 + (3\bar{W}_{1112} - 6\bar{W}_{3123})u^2v \\ + (3\bar{W}_{1113} - 3\bar{W}_{3133})u^2 - 3\bar{W}_{3223}uv^2 - \bar{W}_{3222}uv^3 + 3\bar{W}_{1122}uv^2 + (6\bar{W}_{1123} - 3\bar{W}_{3233})uv \\ + (3\bar{W}_{1133} - \bar{W}_{3333})u + \bar{W}_{1222}v^3 + 3\bar{W}_{1223}v^2 + 3\bar{W}_{1233}v + \bar{W}_{1333} = 0, \\ -\bar{W}_{3111}u^3v + \bar{W}_{2111}u^3 - 3\bar{W}_{3112}u^2v^2 + (3\bar{W}_{2112} - 3\bar{W}_{3113})u^2v + 3\bar{W}_{2113}u^2 - 3\bar{W}_{3122}uv^3 \\ + (3\bar{W}_{2122} - 6\bar{W}_{3123})uv^2 + (6\bar{W}_{2123} - 3\bar{W}_{3133})uv + 3\bar{W}_{2133}u + 3\bar{W}_{2223}v^2 - \bar{W}_{3222}v^4 \\ + (\bar{W}_{2222} - 3\bar{W}_{3223})v^3 - 3\bar{W}_{3233}v^2 + (3\bar{W}_{2233} - \bar{W}_{3333})v + \bar{W}_{2333} = 0. \end{cases}$$
(11)

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

Proof. The conclusion in (a) follows from (7) directly.

If $x_2 \neq 0$ and $x_3 = 0$, then (7) becomes

$$\begin{split} \bar{W}_{1111}x_1^3 + 3\bar{W}_{1112}x_1^2x_2 + 3\bar{W}_{1122}x_1x_2^2 + \bar{W}_{1222}x_2^3 &= \lambda x_1, \\ \bar{W}_{2111}x_1^3 + 3\bar{W}_{2112}x_1^2x_2 + 3\bar{W}_{2122}x_1x_2^2 + \bar{W}_{2222}x_2^3 &= \lambda x_2, \\ \bar{W}_{3111}x_1^3 + 3\bar{W}_{3112}x_1^2x_2 + 3\bar{W}_{3122}x_1x_2^2 + \bar{W}_{3222}x_2^3 &= 0, \\ D_{11}x_1^2 + 2D_{12}x_1x_2 + D_{22}x_2^2 &= 1. \end{split}$$

Let $t = x_1/x_2$. From the first three equations, we have Eq. (8). By the fourth equation, we have (9). This proves (b). If $x_3 \neq 0$, then (7) becomes

From the first three equations, one has

$$\begin{cases} -\bar{W}_{3111x_1}^4 - 3\bar{W}_{3112x_1}^3x_2 + (\bar{W}_{1111} - 3\bar{W}_{3113})x_1^3x_3 - 3\bar{W}_{3122x_1}^2x_2^2 + (3\bar{W}_{1112} - 6\bar{W}_{3123})x_1^2x_2x_3 \\ + (3\bar{W}_{1113} - 3\bar{W}_{3133})x_1^2x_3^2 - 3\bar{W}_{3223}x_1x_2^2x_3 - \bar{W}_{3222}x_1x_2^3 + 3\bar{W}_{1122}x_1x_2^2x_3 + (6\bar{W}_{1123} - 3\bar{W}_{3233})x_1x_3^2 + \bar{W}_{1222x_2}^3x_3 + 3\bar{W}_{1223}x_2^2x_3^2 + 3\bar{W}_{1233}x_2x_3^3 + \bar{W}_{1333}x_4^3 = 0, \\ -\bar{W}_{3111x_1}^3x_2 + \bar{W}_{2111x_1}^3x_3 - 3\bar{W}_{3112}x_1^2x_2^2 + (3\bar{W}_{2112} - 3\bar{W}_{3113})x_1^2x_2x_3 + 3\bar{W}_{2113}x_1^2x_3^2 - 3\bar{W}_{3122}x_1x_2^3 + (6\bar{W}_{2123} - 3\bar{W}_{3133})x_1x_2x_3^2 + (3\bar{W}_{2122} - 6\bar{W}_{3123})x_1x_2^2x_3 + (6\bar{W}_{2123} - 3\bar{W}_{3133})x_1x_2x_3^2 + 3\bar{W}_{2133}x_1x_3^3 + 3\bar{W}_{2223}x_2x_3^2 - \bar{W}_{3222}x_2^4 + (\bar{W}_{2222} - 3\bar{W}_{3223})x_2^3x_3 - 3\bar{W}_{3233}x_2^2x_3^2 + (3\bar{W}_{2233} - \bar{W}_{3333})x_2x_3^3 + \bar{W}_{2333}x_3^4 = 0. \end{cases}$$

Let $u = x_1/x_3$ and $v = x_2/x_3$. Then, (11) follows. By the fourth equation of (12), we have (10). Then conclusion (c) follows now.

We regard the polynomial equation system (11) as equations of u. We may write it as

$$\begin{cases} \alpha_0 u^4 + \alpha_1 u^3 + \alpha_2 u^2 + \alpha_3 u + \alpha_4 = 0\\ \beta_0 u^3 + \beta_1 u^2 + \beta_2 u + \beta_3 = 0, \end{cases}$$

where $\alpha_0, \ldots, \alpha_4, \beta_0, \ldots, \beta_3$ are polynomials of v, which can be calculated by (11). It has complex solutions if and only if its resultant vanishes [2]. By the Sylvester theorem [2], its resultant is equal to the determinant of the following 7×7 matrix:

α_0	α_1	α_2	α_3	α_4	0	0 \	
0	α_0	α_1	α_2	α3	α_4	0	
0	0	$lpha_0$	α_1	α_2	α3	α_4	
β_0	β_1	β_2	β_3	0	0	0	,
0	β_0	β_1	β_2	β_3	0	0	
0	0	β_0	β_1	β_2	β_3	0	
0/	0	0	β_0	β_1	β_2	β_3	

which is a one-dimensional polynomial of v.

To find the approximate solutions of all the real roots of a one-dimensional polynomial, we can use the following Sturm Theorem [7].

Theorem 5. Let ψ be a nonconstant polynomial with real coefficients and let c_1 and c_2 be two real numbers such that $c_1 < c_2$ and $\psi(c_1)\psi(c_2) \neq 0$. The sequence $\psi_0, \psi_1, \ldots, \psi_l$ defined by

 $\psi_0 = \psi, \qquad \psi_1 = \psi', \qquad \psi_{i+1} = -\psi_{i-1} \mod \psi_i, \quad i = 1, 2, \dots, l$

and $\psi_{l+1} \equiv 0$ is called a sequence of Sturm. Denote by v(x) the number of changes of signs in the sequence $\psi_0(x), \psi_1(x), \dots, \psi_l(x)$. Then the number of distinct real roots of ψ on the interval (c_1, c_2) is equal to $v(c_1) - v(c_2)$.

We may find the approximate solutions of all the real roots of this one-dimensional polynomial such that their differences with the exact solutions are within a given error bound. We then substitute them to (11) to find the corresponding approximate real solutions of u. Correspondingly, approximate values of all the D-eigenvalue and their D-eigenvectors can be obtained.

4. A numerical example

In this section, we give a numerical example of *D*-eigenvalues. This example is 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. This example is taken from the white matter.

The diffusion tensor D is

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

	<i>x</i> ₁	<i>x</i> ₂	<i>x</i> ₃	$\lambda \times 10^{-7}$	АКС
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

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

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

Using the method provided in Section 3, we compute all the D-eigenvalues of W, and the associated eigenvectors, which are listed in Table 1.

We see that $\nu = 12$, $\lambda_{\min} = -1.2420 \times 10^7$, $\lambda_{\max} = 5.3545 \times 10^7$ and $M_K = 2.0499 \times 10^7$. We then can calculate that $FA_K = 0.6741$.

In [13], more analysis on this example and another example on gray matter is given.

5. Further discussions

In this paper, we introduced *D*-eigenvalues for a diffusion kurtosis tensor and presented their computation methods. We hope that this discussion in mathematics can be useful in medical engineering. We wonder if they have more general implications in the other fields of engineering and physics. There are some questions for further research:

1. We assume that the diffusion tensor D is positive definite. Is there a practical situation where D is not positive definite? If so, what can we do in such a case?

2. Does ν , the number of the *D*-eigenvalues of *W*, have any practical meaning?

3. In the irregular case, how can we estimate the number of the *D*-eigenvalues?

4. How can we estimate the error bounds of the approximate solutions of *D*-eigenvalues and *D*-eigenvectors obtained in the last section?

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