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THE MEASURE OF DIFFUSION SKEWNESS AND KURTOSIS IN MAGNETIC RESONANCE IMAGING

Xinzhen Zhang, Chen Ling*, Liqun Qi† and Ed Xuekui Wu‡

This paper is dedicated to the memory of Professor Alex Rubinov.

Abstract: The diffusion tensor imaging (DTI) model is an important magnetic resonance imaging (MRI) model in biomedical engineering. It assumes that the water molecule displacement distribution is a Gaussian function. However, water movement in biological tissue is often non-Gaussian and this non-Gaussian behavior may contain useful biological and clinical information. In order to overcome this drawback, a new MRI model, the generalized diffusion tensor imaging (GDTI) model, was presented in [8]. In the GDTI model, even order tensors reflect the magnitude of the signal, while odd order tensors reflect the phase of the signal. In this paper, we propose to use the apparent skewness coefficient (ASC) value to measure the phase of non-Gaussian signals. We prove that the ASC values are invariant under rotations of co-ordinate systems. We discuss some further properties of the diffusion kurtosis tensor and present some preliminary numerical experiments for calculating the ASC values.

Key words: *generalized diffusion tensor imaging, signal processing, skewness, kurtosis, eigenvalues*

Mathematics Subject Classification: *90C90, 15A72*

1 Introduction

The diffusion tensor imaging (DTI) model is an important magnetic resonance imaging (MRI) model in biomedical engineering. It has wide biological and clinical applications [3]. For example, it may be used to study the properties of water molecule diffusion in the brain, particularly for white matter fibers. Such properties may be used to detect abnormalities and diseases in such tissues [1, 2]. In the DTI model, one needs assume a perfect Gaussian distribution for the water molecule movement [3], but water in biological structures often shows non-Gaussian diffusion behavior, which affects the use of the DTI model.

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In order to overcome the drawback of the DTI model, described above, Liu et al. [8] proposed a so-called **generalized diffusion tensors imaging** (GDTI) model as follows

$$\begin{aligned}
\ln\left(\frac{S(b)}{S(0)}\right) &= -\sum_{i_1,i_2=1}^{3} D^{(2)}_{i_1i_2} b^{(2)}_{i_1i_2} + \sum_{i_1,\cdots,i_4=1}^{3} D^{(4)}_{i_1\cdots i_4} b^{(4)}_{i_1\cdots i_4} + \cdots \\
&\quad +(-1)^n \sum_{i_1,\cdots,i_{2n}=1}^{3} D^{(2n)}_{i_1\cdots i_{2n}} b^{(2n)}_{i_1\cdots i_{2n}} + \cdots \\
&\quad +j\left(-\sum_{i_1,i_2,i_3=1}^{3} D^{(3)}_{i_1i_2i_3} b^{(3)}_{i_1i_2i_3} + \sum_{i_1,\cdots,i_5=1}^{3} D^{(5)}_{i_1\cdots i_5} b^{(5)}_{i_1\cdots i_5} + \cdots \right. \\
&\quad \left. +(-1)^n \sum_{i_1,\cdots,i_{2n+1}=1}^{3} D^{(2n+1)}_{i_1\cdots i_{2n+1}} b^{(2n+1)}_{i_1\cdots i_{2n+1}} + \cdots \right),
\end{aligned} \tag{1.1}$$

to characterize the non-Gaussian diffusion of the water molecules in tissues, where $S(0)$ and $S(b)$ are the transverse magnetization measured at the echo (TE) in the absence and presence of diffusion gradient, respectively. Here, j is the square root of -1, and $D^{(n)}$ $(n \geq 2)$ are n-th order coefficient tensors which can be determined by using some common statistical methods such as the least square estimate method and Monte-Carlo simulations.

It is not difficult to see that the tensors $b^{(n)}$ $(n \geq 2)$ in (1.1) are functions of the direction, the magnitude, and the timing of the diffusion-encoding gradients. More precisely, if the magnetic field gradient is a constant vector over the considered time, by [8], the element $b^{(n)}_{i_1i_2\cdots i_n}$ of tensor $b^{(n)}$ can be written as

$$b^{(n)}_{i_1i_2\cdots i_n} = (\gamma g\delta)^n \left(\Delta - \frac{n-1}{n+1}\delta\right) x_{i_1}x_{i_2}\cdots x_{i_n}, \quad i_1, i_2, \cdots, i_n = 1, 2, 3, \tag{1.2}$$

where $x = (x_1, x_2, x_3)^T \in \Re^3$ is the considered direction, Δ is the separation time of the two diffusion gradients, δ is the duration of each gradient lobe, and g is an appropriate positive number. From (1.1), it is obvious that in the case of Gaussian diffusion, all the tensors $D^{(n)}$ of orders higher than two are zero. For non-Gaussian diffusion, however, those higher order tensors become significant, and it is important to recognize that the higher order terms in (1.1) have to be considered in such situations.

From (1.1), we can also see that the real part of the logarithmic signal is solely determined by the even order tensors and only affects the magnitude of the signal, while the imaginary part is completely governed by odd order tensors and only affects the phase of the signal. This shows that if we consider the diffusion behavior of the non-Gaussian signal with the asymmetry, the DTI model may fail to identify the underlying structure [9]. This point is even clearer for the one modeled by Phantom 4 in [8]. We refer readers to [5, 6, 13, 14] and references therein for non-Gaussian diffusion with the symmetry.

In this paper, we consider the approximation of (1.1) as follows

$$\ln\left(\frac{S(b)}{S(0)}\right) = -\sum_{i_1,i_2=1}^{3} D^{(2)}_{i_1i_2} b^{(2)}_{i_1i_2} + \sum_{i_1,i_2,i_3,i_4=1}^{3} D^{(4)}_{i_1i_2i_3i_4} b^{(4)}_{i_1i_2i_3i_4} - j \sum_{i_1,i_2,i_3=1}^{3} D^{(3)}_{i_1i_2i_3} b^{(3)}_{i_1i_2i_3}, \tag{1.3}$$

which can be obtained by truncating (1.1) to the fourth order tensor and contains useful information of the signal. Then the first two terms of (1.3) are related to the magnitude of the signal and the last term of (1.3) is related to the phase of the signal. The second order tensor $D^{(2)}$ is the **diffusion tensor**. We call the third order $D^{(3)}$ and the fourth order tensor $D^{(4)}$ in (1.3) the **diffusion skewness (DS) tensor** and the **diffusion kurtosis (DK) tensor** respectively. It is important to note that the values $D^{(2)}_{i_1i_2}$, $D^{(3)}_{i_1i_2i_3}$ and $D^{(4)}_{i_1i_2i_3i_4}$ in (1.3) are not independent of the co-ordinate system. When the co-ordinate system is rotated, these values will be changed. To understand the biological and clinical meaning of the corresponding tensors in (1.3), we have to measure and calculate some quantities and parameters which are independent from co-ordinate system choices. The main invariants of the diffusion tensor $D^{(2)}$ are its eigenvalues, which have already been widely used in the DTI technique [3]. In [16], Qi et al. introduced D-eigenvalues for a DK tensor $D^{(4)}$. Some important invariants related to $D^{(4)}$ were identified there. Moreover, a method for calculating D-eigenvalues was presented in [16]. Here we study the quantities and parameters associated with the DS tensor $D^{(3)}$ in (1.3), which include the largest and the smallest **apparent skewness coefficients** (ASC) values, their computation formulas and relationships, and some further properties of the invariants of $D^{(4)}$.

In Section 2, we discuss some further properties of the invariants of $D^{(4)}$. In Section 3, based on the concept of Z-eigenvalues of tensors [11], we introduce the ASC values, and show that they are invariant under co-ordinate rotations and may have important biological and clinical meanings.

In Section 4, we describe numerical methods to calculate the ASC values and the **apparent kurtosis coefficients** (AKC) values. In Section 5, we provide some numerical examples for calculating ASC values. Some final conclusions are made in Section 6.

2 The AKC Values

In this section, we first summarize the concept and properties of AKC values, then further discuss some properties of the D-eigenvalues and Kelvin eigenvalues of $D^{(4)}$. To this end, let us write

$$D = (\gamma g\delta)^2 \left(\Delta - \frac{1}{3}\delta\right) D^{(2)}, \tag{2.1}$$

and

$$W = (\gamma g\delta)^4 \left(\Delta - \frac{3}{5}\delta\right) D^{(4)}. \tag{2.2}$$

Then the apparent diffusion coefficient (ADC) [3]

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

In practice, D is positive definite. Let the eigenvalues of D be $\alpha_1 \geq \alpha_2 \geq \alpha_3 > 0$. Then the mean diffusivity [3] can be calculated by

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

As [11, 16], we denote Dx and Wx^3 as two vectors in $\Re^3$ with their ith component as

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

and

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

respectively, for $i = 1,2,3$. In [16], Qi et. al introduced the following concept of D-eigenvalues and D-eigenvectors of W, which is a generalization of Z-eigenvalues and Z-eigenvectors presented in [11].

Definition 2.1. A real number λ is said to be a D-eigenvalue of W, if there exists a real vector x such that

$$\begin{cases} Wx^3 = \lambda Dx, \\ Dx^2 = 1. \end{cases} \tag{2.3}$$

The real vector x is called the D-eigenvector of W associated with the D-eigenvalue λ.

Based on this definition, a key formula for the tensor W is as follows:

$$K_{app}(x) = \frac{M_D^2}{D_{app}^2} Wx^4, \tag{2.4}$$

where $K_{app}(x)$ is the AKC value at the direction x, and

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

Denote the largest and the smallest AKC values as $K_{\max}$ and $K_{\min}$ respectively. Then we have the following theorems which were proved in [16].

Theorem 2.2. *D-eigenvalues of W are real numbers and always exist. If x is a D-eigenvector associated with a D-eigenvalue λ, then*

$$\lambda = Wx^4.$$

Denote the largest and the smallest D-eigenvalues of W as $\lambda_{\max}^D$ and $\lambda_{\min}^D$ respectively. Then the largest AKC value is

$$K_{\max} = M_D^2 \lambda_{\max}^D, \tag{2.5}$$

and the smallest AKC value is

$$K_{\min} = M_D^2 \lambda_{\min}^D. \tag{2.6}$$

Theorem 2.3. *The D-eigenvalues of W are invariant under rotations of co-ordinate systems.*

By these two theorems, we know that $K_{\max}$ and $K_{\min}$ are also invariants of W. In the rest of this section, we discuss some further properties of eigenvalues of W.

In [4], a 6×6 symmetric matrix is associated with a fourth order three dimensional symmetric tensor. The eigenvalues of that matrix are also invariants of that tensor. This theory can be traced back to Kelvin 150 years ago [17]. For tensor W, we call the six eigenvalues of the 6 matrix associated with it **Kelvin eigenvalues** of W. Are there any relations between D-eigenvalues and Kelvin eigenvalues? By the definitions of D-eigenvalues and Kelvin eigenvalues [4], the following proposition holds.

Proposition 2.4. *Let W be a fourth order three dimensional fully symmetric tensor, and let σ be a Kelvin eigenvalue of W, associated with a Kelvin eigentensor X. If there exists a vector $x \in \Re^3$ such that $X = xx^T$, then σ is a D-eigenvalue of W.*

Proposition 2.5. *Let $\sigma_1, \sigma_2, \cdots, \sigma_6$ be 6 Kelvin eigenvalues of W. Suppose $D = I$. Then we have*

$$-\sum_{m=1}^{6}(-\sigma_m)_+ \le \lambda_{\min}^D \le \lambda_{\max}^D \le \sum_{m=1}^{6}(\sigma_m)_+,$$

where $(a)_+ = \max\{a, 0\}$.

Proof. Is is easy to verify that we have the spectral decomposition of W as follows

$$W = \sum_{m=1}^{6} \sigma_m E^m \otimes E^m, \tag{2.7}$$

where $\otimes$ denotes the outer tensor product,

$$E^m = \begin{pmatrix} \varepsilon_{11}^m & \frac{1}{\sqrt{2}}\varepsilon_{12}^m & \frac{1}{\sqrt{2}}\varepsilon_{13}^m \\ \frac{1}{\sqrt{2}}\varepsilon_{12}^m & \varepsilon_{22}^m & \frac{1}{\sqrt{2}}\varepsilon_{23}^m \\ \frac{1}{\sqrt{2}}\varepsilon_{13}^m & \frac{1}{\sqrt{2}}\varepsilon_{23}^m & \varepsilon_{33}^m \end{pmatrix},$$

and $\varepsilon^m = (\varepsilon_{11}^m, \varepsilon_{22}^m, \varepsilon_{33}^m, \varepsilon_{12}^m, \varepsilon_{13}^m, \varepsilon_{23}^m)^T$ is the mth normalized Kelvin eigenvector of W [4]. It is clear that for each m, E^m is a symmetric matrix satisfying $\mathrm{trace}(E^m)^2 = 1$, which implies that $\mu_{m1}^2 + \mu_{m2}^2 + \mu_{m3}^2 = 1$, where $\mu_{m1} \le \mu_{m2} \le \mu_{m3}$ are three eigenvalues of E^m. By (2.7), we have that for any $x = (x_1, x_2, x_3)^T$,

$$\begin{aligned} Wx^4 &= \sum_{i,j,l,k}^{3} W_{ijkl}x_ix_jx_kx_l \\ &= \sum_{m=1}^{6} \sigma_m (x^T E^m x)^2. \end{aligned} \tag{2.8}$$

It is well known that $\mu_{m1} \le x^T E^m x \le \mu_{m3}$ for any $m = 1, \cdots, 6$. This implies that $0 \le (x^T E^m x)^2 \le \max\{\mu_{m1}^2, \mu_{m3}^2\} \le 1$. Therefore, by (2.8), we obtain the desired result and complete the proof. □

Now we discuss the independence of eigenvalues of fourth order three dimensional tensor. We first give the following definition.

Definition 2.6. A set S consisted of the functions

$$y_i = f_i(x_1, x_2, \cdots, x_n), \quad i = 1, 2, \cdots, m, \tag{2.9}$$

which are defined on the region Ω in $\Re^n$, is said to be functionally dependent on Ω, if there exist an index i_0 and a function φ defined on an appropriate region in $\Re^{m-1}$, such that

$$\begin{aligned} y_{i_0} \equiv\ & \varphi(f_1(x_1, x_2, \cdots, x_n), f_2(x_1, x_2, \cdots, x_n), \cdots, \\ & f_{i_0-1}(x_1, x_2, \cdots, x_n), f_{i_0+1}(x_1, x_2, \cdots, x_n), \cdots, f_m(x_1, x_2, \cdots, x_n)) \end{aligned}$$

holds for any $(x_1, x_2, \cdots, x_n) \in \Omega$. If for any sub-region Ω' of Ω, there are no i_0 and such function φ that

$$y_{i_0} \equiv \varphi(y_1, y_2, \cdots, y_{i_0-1}, y_{i_0+1}, \cdots, y_m)$$

holds on Ω', then the function set S is said to be functionally independent on Ω.

For the functional independence, we have the following theorem.

Theorem 2.7. *Suppose that $m \leq n$ and there exists an mth order determinant $|A|$ in the Jacobian matrix of the functions set (2.9) such that $|A| \neq 0$ holds on Ω. Then the functions set S is functionally independent on Ω.*

It is important to note that the trace Π_K of W in the sense of Kelvin is an important invariant, which characterizes the average AKC value on a spherical surface and has physics significance. In addition, the largest D-eigenvalue $\lambda^D_{\max}$ and the smallest D-eigenvalue $\lambda^D_{\min}$ of W play an important role in the diffusion analysis of the water molecule in biological tissue. From Proposition 2.5, we see that the largest D-eigenvalue and the smallest D-eigenvalue of W can be estimated with an interval determined by the Kelvin eigenvalues of W. However, this result does not mean that there must be some functional dependence between the largest (smallest) D-eigenvalues and Kelvin eigenvalues of W. In fact, the following example shows that both $\{\lambda^D_{\max}, \lambda^D_{\min}, \Pi_K\}$ and $\{\lambda^D_{\max}, \lambda^D_{\min}, \sigma_{\max}, \sigma_{\min}\}$ are functionally independent on a considered region, where $\sigma_{\max}$ and $\sigma_{\min}$ denote the largest and smallest Kelvin eigenvalue of W, respectively.

Example 2.1 Let W be a fourth order three dimensional fully symmetric tensor with $W_{1111} = t_1$, $W_{2222} = t_2$, $W_{3333} = t_3$, $W_{1122} = t_4$ and its other elements are zero, and let $D = I$. Consider the case where $0 < t_1 < t_3 < 3t_4 < t_2$, $t_1 < t_4$ and $t_1 t_2 < t_4^2$. By Definition 2.1, it is easy to obtain that the D-eigenvalues of W are as follows

$$\lambda_1 = t_1, \quad \lambda_2 = t_2, \quad \lambda_3 = t_3, \quad \lambda_4 = \frac{t_1 t_3}{t_1 + t_3}, \quad \lambda_5 = \frac{t_2 t_3}{t_2 + t_3}.$$

Under the given conditions, it is easy to see that the largest and smallest D-eigenvalues of W are

$$\lambda^D_{\max} = F_1(t_1, t_2, t_3, t_4) := t_2 \quad \text{and} \quad \lambda^D_{\min} = F_2(t_1, t_2, t_3, t_4) := \frac{t_1 t_3}{t_1 + t_3},$$

respectively. On the other hand, it is clear that the trace Π_K in sense of Kelvin

$$\Pi_K = F_3(t_1, t_2, t_3, t_4) := t_1 + t_2 + t_3 + 2t_4.$$

Moreover, by direct computation, we obtain that the set consisted of all Kelvin eigenvalues of W is

$$\left\{ \frac{t_1 + t_2 + \sqrt{(t_1 - t_2)^2 + 4t_4^2}}{2}, \frac{t_1 + t_2 - \sqrt{(t_1 - t_2)^2 + 4t_4^2}}{2}, t_3, 2t_4, 0, 0 \right\},$$

which implies that the largest and smallest Kelvin eigenvalues of W are

$$\sigma_{\max} = F_4(t_1, t_2, t_3, t_4) := \frac{t_1 + t_2 + \sqrt{(t_1 - t_2)^2 + 4t_4^2}}{2}$$

and

$$\sigma_{\min} = F_5(t_1, t_2, t_3, t_4) := \frac{t_1 + t_2 - \sqrt{(t_1 - t_2)^2 + 4t_4^2}}{2},$$

respectively. Based on these above, it is easy to verify that the Jacobian matrices of $\hat{F} := (F_1, F_2, F_3)$ and $\tilde{F} := (F_1, F_2, F_4, F_5)$ are

$$\nabla \hat{F}(t_1, t_2, t_3, t_4) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{t_3^2}{(t_1 + t_3)^2} & 0 & \frac{t_1^2}{(t_1 + t_3)^2} & 0 \\ 1 & 1 & 1 & 2 \end{pmatrix}$$

and

$$\nabla \tilde{F}(t_1, t_2, t_3, t_4) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{t_3^2}{(t_1+t_3)^2} & 0 & \frac{t_1^2}{(t_1+t_3)^2} & 0 \\ \frac{1}{2}\left(1 + \frac{t_1 - t_2}{\sqrt{(t_1-t_2)^2+4t_4^2}}\right) & \frac{1}{2}\left(1 - \frac{t_1 - t_2}{\sqrt{(t_1-t_2)^2+4t_4^2}}\right) & 0 & \frac{2t_4}{\sqrt{(t_1-t_2)^2+4t_4^2}} \\ \frac{1}{2}\left(1 - \frac{t_1 - t_2}{\sqrt{(t_1-t_2)^2+4t_4^2}}\right) & \frac{1}{2}\left(1 + \frac{t_1 - t_2}{\sqrt{(t_1-t_2)^2+4t_4^2}}\right) & 0 & -\frac{2t_4}{\sqrt{(t_1-t_2)^2+4t_4^2}} \end{pmatrix},$$

respectively. It is easy to see that for $\hat{F}$ and $\tilde{F}$, the conditions required in Theorem 2.7 are satisfied. Hence, we know that both $\{\lambda^D_{\max}, \lambda^D_{\min}, \Pi_K\}$ and $\{\lambda^D_{\max}, \lambda^D_{\min}, \sigma_{\max}, \sigma_{\min}\}$ are functionally independent on $\Omega := \{(t_1, t_2, t_3, t_4) \mid 0 < t_1 < t_3 < 3t_4 < t_2,\ t_1 < t_4 \text{ and } t_1 t_2 < t_4^2\}$.

3 The ASC Values

As mentioned in Section 1, we may use ASC value to characterize the phase of the magnetic resonance signal in biological tissues. Let us write

$$P = (\gamma g \delta)^3 \left(\Delta - \frac{2}{4}\delta\right) D^{(3)}, \tag{3.1}$$

which is a third order three dimensional fully symmetric tensor. Here, P has ten independent elements because of symmetry. For those elements of P which are equal to each other, we use the element P_{ijk} with $i \leq j \leq k$ to represent them. That is, if we say that $P_{122} = 4$, this automatically implies that $P_{212} = P_{221} = 4$. Then, the ten independent elements of P are $P_{111}; P_{222}; P_{333}; P_{112}; P_{113}; P_{223}; P_{122}; P_{133}; P_{233}; P_{123}$. We call $P_{111}; P_{222}; P_{333}$ the diagonal elements of P. We denote $S_{app}(x)$ the apparent skewness coefficient at the direction x as follows

$$S_{app}(x) = \frac{Px^3}{\|x\|^3}, \tag{3.2}$$

where

$$Px^3 \equiv \sum_{i,j,k=1}^{3} P_{ijk} x_i x_j x_k.$$

We denote Px^2 as a vector in $\Re^3$ with its ith component as

$$(Px^2)_i = \sum_{j,k=1}^{3} P_{ijk} x_j x_k,$$

for $i = 1, 2, 3$. Denote the largest and the smallest ASC values as $S_{\max}$ and $S_{\min}$ respectively. Then

$$S_{\max} = \begin{array}{ll} \max & Px^3 \\ \text{s.t} & \|x\|^2 = 1, \end{array} \tag{3.3}$$

and

$$S_{\min} = \begin{array}{ll} \min & Px^3 \\ \text{s.t} & \|x\|^2 = 1. \end{array} \tag{3.4}$$

The critical points of (3.3) and (3.4) satisfy the following system for some $\lambda \in \Re$ and $x \in \Re^3$:

$$\begin{cases} Px^2 = \lambda x, \\ \|x\|^2 = 1. \end{cases} \tag{3.5}$$

A real number λ satisfying (3.5) with a real vector x is called a Z-eigenvalue of P, and the real vector x is called the Z-eigenvector of P associated with the Z-eigenvalue λ [11]. We have the following two theorems which can be proved by a similar way to that in [16].

Theorem 3.1. *Z-eigenvalues always exist. If x is a Z-eigenvector associated with a Z-eigenvalue λ, then*

$$\lambda = Px^3.$$

Denote the largest and the smallest Z-eigenvalues of P as $\lambda^Z_{\max}$ and $\lambda^Z_{\min}$ respectively. Then the largest ASC value is

$$S_{\max} = \lambda^Z_{\max}, \tag{3.6}$$

and the smallest ASC value is

$$S_{\min} = \lambda^Z_{\min}. \tag{3.7}$$

Theorem 3.2 ([12]). *The Z-eigenvalues of P are invariant under rotations of co-ordinate systems.*

Remark 3.3. By these two theorems, $S_{\max}$ and $S_{\min}$ are also invariants of P, and can be calculated by a similar method to that given in [16], which will be presented in Section 4. On the other hand, from the definition of Z-eigenvalues and Z-eigenvectors, we know that λ is a Z-eigenvalue of P with its an eigenvector x if and only if $-\lambda$ is a Z-eigenvalue of P with the associated eigenvector $-x$. Hence, $\lambda^Z_{\min} = -\lambda^Z_{\max}$.

Denote the unit sphere as

$$\Xi := \{x \in \Re^3 \ : \ x_1^2 + x_2^2 + x_3^2 = 1\}.$$

Then the average ASC value over the Ξ is defied as

$$M_\Xi = \frac{1}{\Xi} \int\int_\Xi S_{\mathrm{app}}(x) dA = \frac{1}{4\pi} \int\int_\Xi \frac{Px^3}{\|x\|^3} dA, \tag{3.8}$$

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

Noting the fact that P is an odd order full symmetric tensor, it is obvious that for any closed surface Λ with symmetry about the origin, the average ASC value over Λ is equal to zero. Specially, it holds that $M_\Xi = 0$.

4 Computation of the ASC and AKC Values

In this section, we describe direct methods to find all Z-eigenvalues of P and D-eigenvalues of W, respectively. Then $S_{\max}$, $S_{\min}$, $K_{\max}$ and $K_{\min}$ can be calculated.

The first method is used to find all the Z-eigenvalues of P. The key idea here is to reduce the three variable system (3.5) 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 [7] to solve this system.

Based on the consideration above, we state the following theorem which generalizes Theorem 3 in [15] and can be proved in a similar way to that used in [16] .

Theorem 4.1. *(a) If $P_{211} = P_{311} = 0$, then $x = (\pm 1, 0, 0)^T$ are two Z-eigenvector of P associated with the Z-eigenvalue $\lambda = \pm P_{111}$, respectively.*

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

$$\begin{cases} P_{211}t^3 + (2P_{212} - P_{111})t^2 + (P_{222} - 2P_{112})t - P_{122} = 0, \\ P_{311}t^2 + 2P_{312}t + P_{322} = 0, \end{cases} \tag{4.1}$$

$$x = \pm \frac{1}{\sqrt{t^2+1}} (t, 1, 0)^T \tag{4.2}$$

is a Z-eigenvector of P with the Z-eigenvalue $\lambda = Px^3$.

(c) $\lambda = Px^3$ and

$$x = \frac{\pm (u, v, 1)^T}{\sqrt{u^2 + v^2 + 1}} \tag{4.3}$$

constitute a Z-eigenpairs of P, where u and v are a real solution of the following polynomial equations:

$$\begin{cases} -P_{311}u^3 - 2P_{312}u^2v - P_{322}uv^2 + (P_{111} - 2P_{313})u^2 + 2(P_{112} - P_{323})uv \\ \qquad + P_{122}v^2 + (2P_{113} - P_{333})u + 2P_{123}v + P_{133} = 0, \\ P_{211}u^2 - P_{311}u^2v - 2P_{312}uv^2 + 2(P_{212} - P_{313})uv + 2P_{213}u - P_{322}v^3 \\ \qquad + (P_{222} - 2P_{323})v^2 + 2(P_{223} - P_{333})v + P_{233} = 0. \end{cases} \tag{4.4}$$

All the Z-eigenpairs of tensor P are given by (a), (b) and (c) if $P_{211} = P_{311} = 0$, and by (b) and (c) otherwise.

We regard the polynomial equation system (4.4) as equations of u. We may write it as

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

where $\alpha_0, \cdots, \alpha_3, \beta_0, \cdots, \beta_2$ are polynomials of v, which can be calculated by (4.4). It has complex solutions if and only if its resultant vanishes [7]. By the Sylvester theorem [7], its resultant is equal to the determinant of the following 5×5 matrix:

$$\begin{pmatrix} \alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 & 0 \\ 0 & \alpha_0 & \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_0 & \beta_1 & \beta_2 & 0 & 0 \\ 0 & \beta_0 & \beta_1 & \beta_2 & 0 \\ 0 & 0 & \beta_0 & \beta_1 & \beta_2 \end{pmatrix},$$

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 [10].

Theorem 4.2. *Let ψ be a nonconstant polynomial of degree l, 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 $\psi_0, \psi_1, \cdots, \psi_l$ defined by*

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

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 $\psi_0(x), \psi_1(x), \cdots, \psi_l(x)$. 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 (4.4) to find the corresponding approximate real solutions of u. Correspondingly, approximate values of all the Z-eigenvalues and Z-eigenvectors can be obtained. Based on this, we can obtain the largest and smallest ASC values.

The second method is used to find all the D-eigenvalues of W, which is similar as above and is based on the following theorem given in [16].

Theorem 4.3. *Let $\bar{W}$ be a fourth order three dimensional tensor such that its entries satisfy $\bar{W}_{ijkl} = \sum_{h=1}^{3} \bar{d}_{ih} W_{ijkl}$ for $i,j,k,l = 1,2,3$, where $\bar{d}_{ih}$ is the ith row hth column element in the inverse D^{-1} of D. Then we have*

(a) If $\bar{W}_{2111} = \bar{W}_{3111} = 0$, then $\lambda = \frac{\bar{W}_{111}}{D_{11}}$ is a D-eigenvalue of W with a D-eigenvector $x = (\pm\sqrt{\frac{1}{D_{11}}}, 0, 0)^T$.

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

$$\begin{cases} -\bar{W}_{2111}t^4 + (\bar{W}_{1111} - 3\bar{W}_{2112})t^3 + 3(\bar{W}_{1112} - \bar{W}_{2122})t^2 \\ +(3\bar{W}_{1122} - \bar{W}_{2222})t + \bar{W}_{1222} = 0, \\ \bar{W}_{3111}t^3 + 3\bar{W}_{3112}t^2 + 3\bar{W}_{3122}t + \bar{W}_{3222} = 0, \end{cases} \tag{4.5}$$

$$x = \pm\frac{1}{\sqrt{D_{11}t^2 + 2D_{12}t + D_{22}}}(t,1,0)^T \tag{4.6}$$

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

(c) $\lambda = Wx^4$ and

$$x = \frac{\pm(u,v,1)^T}{\sqrt{D_{11}u^2 + 2D_{12}uv + 2D_{13}u + D_{22}v^2 + 2D_{23}v + D_{33}}} \tag{4.7}$$

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

$$\begin{cases} -\bar{W}_{3111}u^4 - 3\bar{W}_{3112}u^3v + (W_{1111} - 3\bar{W}_{3113})u^3 - 3\bar{W}_{3122}u^2v^2 \\ +(3\bar{W}_{1112} - 6\bar{W}_{3123})u^2v + +(3\bar{W}_{1113} - 3\bar{W}_{3133})u^2 \\ -3\bar{W}_{3223}uv^2 - \bar{W}_{3222}uv^3 + 3\bar{W}_{1122}uv^2 + (6W_{1123} - 3\bar{W}_{3233})uv \\ +(3\bar{W}_{1133} - \bar{W}_{3333})u + \bar{W}_{1222}v^3 + 3\bar{W}_{1223}v^2 + 3\bar{W}_{1233}v + \bar{W}_{1333} = 0, \\ -\bar{W}_{3111}u^3v + \bar{W}_{2111}u^3 - 3\bar{W}_{3112}u^2v^2 + (3\bar{W}_{2112} - 3\bar{W}_{3113})u^2v \\ +3\bar{W}_{2113}u^2 - 3\bar{W}_{3122}uv^3 + (3\bar{W}_{2122} - 6\bar{W}3123)uv^2 \\ +(6\bar{W}_{2123} - 3\bar{W}_{3133})uv + 3\bar{W}_{2133}u + 3\bar{W}_{2223}v^2 - \bar{W}_{3222}v^4 \\ +(W_{2222} - 3\bar{W}_{3223})v^3 - 3\bar{W}_{3233}v^2 + (3\bar{W}_{2233} - \bar{W}_{3333})v + \bar{W}_{2333} = 0. \end{cases} \tag{4.8}$$

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

5 Numerical Examples

In this section, we present preliminary numerical experiments for the DS tensor with the method presented in Section 4. The computation was done on a personal computer (Pentium

IV, 2.8GHz) by running MatlabR2006a. A numerical example for DK tensor can be found in [16]. That example is derived from data of MRI experiments on the white matter of 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.

For the test examples below, we choose the parameters in (1.2) as follows

$$\triangle = 1, \quad \delta = 0.5, \quad g = 1, \quad \gamma = 1.$$

Then the tensor P in (3.1) becomes $P = \frac{3}{32}D^{(3)}$.

By Theorem 4.1, we can obtain all the Z-eigenvalues of P, and the associated eigenvectors. As mentioned in Remark 3.3, $-\lambda$ must be another Z-eigenvalue of it when λ is a Z-eigenvalue of P. Throughout this section, we present only the nonnegative Z-eigenvalues and the corresponding Z-eigenvectors of P in the following tables.

Example 5.1 This example was taken from [8], conducted by Monte-Carlo simulations using computer-synthesized phantoms with a Y-shape tube. The Y-shape tube is asymmetric and the DTI technique fails to identify this structure.

For this example, the ten independent elements of $D^{(3)}$ are $D^{(3)}_{111} = -2.36, D^{(3)}_{112} = 47.9, D^{(3)}_{113} = 0, D^{(3)}_{122} = -0.773, D^{(3)}_{123} = -0.575, D^{(3)}_{133} = 0.282, D^{(3)}_{222} = -28.7, D^{(3)}_{223} = 0, D^{(3)}_{233} = 3.61, D^{(3)}_{333} = 0.488$ in unit of $10^{-8}mm^3/s$.

The numerical results for Example 5.1 are listed in the Table 1.

number	x_1	x_2	x_3	$\lambda \times 10^7$
(1)	0	-1.0000	0	0.2691
(2)	-0.0062	-1.0000	-0.0002	0.2691
(3)	-0.8514	0.5244	0.0097	0.4922
(4)	0.8480	0.5299	-0.0108	0.4548
(5)	-0.0431	0.0557	0.9975	0.0044
(6)	0.0494	-0.0684	0.9964	0.0049

Table 1: Z-eigenvalues and eigenvectors of P in Example 5.1

From Table 1, we can see that there are 12 Z-eigenvalues and corresponding Z-eigenvectors for P, and the largest and smallest Z-eigenvalues of P are 0.4922×10^{-7} and -0.4922×10^{-7}, which attained at $(-0.8514, 0.5244, 0.0097)^T$ and $(0.8514, -0.5244, -0.0097)^T$, respectively. This implies that $S_{\max} = 0.4922 \times 10^{-7}$ and $S_{\min} = -0.4922 \times 10^{-7}$.

In order to illustrate the efficiency of our method, we also calculate the Z-eigenvalues and corresponding Z-eigenvectors of ten third order three dimensional full symmetric tensors which are constructed randomly in the following example.

Example 5.2 The elements of P are drawn by a normal distribution with mean zero and standard deviation one.

Using the method provided in Section 4, we compute all the Z-eigenvalues of P, and the associated eigenvectors. In Table 2, the largest Z-eigenvalue and the corresponding Z-eigenvectors are listed for ten tensors. Moreover, in Table 3, all the nonnegative Z-eigenvalues with corresponding Z-eigenvectors are presented for Tensor 1 in ten tensors.

Tensor	x_1	x_2	x_3	$\lambda^Z_{\max}$
1	-0.5784	0.7896	0.2050	2.1161
2	-0.8364	-0.0495	0.5459	3.2879
3	-0.6272	-0.2393	-0.7411	2.6702
4	-0.0836	-0.8832	-0.5467	2.9957
5	0.7021	-0.6410	0.3100	2.5146
6	-0.7327	0.6778	0.0612	4.1874
7	0.1531	0.5353	0.8307	3.5715
8	0.7981	-0.5944	0.0991	4.2279
9	-0.6308	-0.6893	-0.3563	3.3815
10	-0.2657	0.7381	-0.6201	3.4800

Table 2: The Largest Z-eigenvalues with Z-eigenvectors for ten tensors

number	x_1	x_2	x_3	λ
(1)	-0.3518	-0.9140	0.2020	0.9434
(2)	-0.5784	0.7896	0.2050	2.1161
(3)	-0.4346	-0.6970	-0.5704	1.6851
(4)	0.9455	0.1980	-0.2585	1.4644
(5)	0.0836	-0.5452	0.8341	1.5940
(6)	0.8322	-0.1726	0.5269	0.5171
(7)	0.3823	-0.1797	-0.9064	0.0165

Table 3: Nonnegative Z-eigenvalues and Z-eigenvectors of Tensor 1

6 Final Conclusion

In this paper, we introduced the concept of diffusion skewness in magnetic resonance imaging and discussed the measure of the diffusion skewness and kurtosis. The diffusion skewness and kurtosis provide two dimensionless values for characterizing the phase of the signal in tissues and the degree of non-Gaussian of the diffusion displacement probability distribution, respectively. For the water molecule with Gaussian distribution in biological structures, the skewness and kurtosis are zero. But, for those non-Gaussian signal with asymmetry about the origin, the skewness and the kurtosis have significant values. Based on the Z-eigenvalues and D-eigenvalues of tensor, the methods for calculating the largest (smallest) ASC values and largest (smallest) AKC values were presented. These ASC and AKC values are the principal invariants under rotations of co-ordinate systems and can be calculated in any Cartesian co-ordinate system. For the fourth order three dimensional fully symmetric tensor, we presented some properties of it and discussed the functionally independence for the largest D-eigenvalue, the smallest D-eigenvalue and the trace in sense of Kelvin. We hope that these quantities and properties can be useful for the diffusion analysis of the signal in GDTI practice.

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Xinzhen Zhang
Department of Applied Mathematics
The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong
E-mail address: xzhang@yahoo.cn

Chen Ling
School of Science, Hangzhou Dianzi University
Hangzhou, 310018, China
E-mail address: linghz@hzcnc.com

Liqun Qi
Department of Applied Mathematics
The Hong Kong Polytechnic University
Hung Hom, Kowloon, Hong Kong
E-mail address: maqilq@polyu.edu.hk

Ed Xuekui Wu
Department of Electrical and Electronic Engineering
The University of Hong Kong, Hong Kong
E-mail address: ewu@eee.hku.hk