# POSITIVE DEFINITENESS OF DIFFUSION KURTOSIS IMAGING 

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#### Abstract

Diffusion Kurtosis Imaging (DKI) is a new Magnetic Resonance Imaging (MRI) model to characterize the non-Gaussian diffusion behavior in tissues. In reality, the term $b D_{a p p}-\frac{1}{6} b^{2} D_{a p p}^{2} K_{a p p}$ in the extended Stejskal and Tanner equation of DKI should be positive for an appropriate range of $b$-values to make sense physically. The positive definiteness of the above term reflects the signal attenuation in tissues during imaging. Hence, it is essential for the validation of DKI.

In this paper, we analyze the positive definiteness of DKI. We first characterize the positive definiteness of DKI through the positive definiteness of a tensor constructed by diffusion tensor and diffusion kurtosis tensor. Then, a conic linear optimization method and its simplified version are proposed to handle the positive definiteness of DKI from the perspective of numerical computation. Some preliminary numerical tests on both synthetical and real data show that the method discussed in this paper is promising.


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## 1. Introduction

Magnetic Resonance Imaging (MRI) [6], especially Diffusion Tensor Imaging (DTI), has proved to be powerful when we investigate the anatomical connections of the human nervous system in vivo and non-invasively [2, 4, 5, 6]. However, DTI suffers a great limitation due to its inability of dealing with non-Gaussian diffusion. Hence, serval new models were proposed recently to solve this problem. These include the approaches based on High Angular Resolution Diffusion Imaging (HARDI) techniques: radial basis functions [28, Spherical Harmonics (SH) [10], etc; and the approaches based on some extensions of the Stejskal and Tanner equation: Higher Order Tensors (HOT) [14, 15, 16, 18, Diffusion Kurtosis Imaging (DKI) [12, 13, 17, 24] which is a fourth-order truncation of the HOT model, etc.

Among the above models for dealing with non-Gaussian diffusion, we are interested in DKI here. It has been proved that DKI has the ability to deal with non-Gaussian diffusion [12, 13, 17, 21, 24. One of the key issue in DKI is to handle the diffusion kurtosis tensor in that model [12, 17, 21]. A diffusion kurtosis tensor $W$ is a fourth-order three-dimensional supersymmetric tensor [21, 22]. It has fifteen independent elements $W_{i j k l}$ with $W_{i j k l}$ being invariant for any permutation of its indices $i, j, k, l=1,2,3$ [21]. It comes from the following extended Stejskal and Tanner equation [12, 25]:

$$
\begin{equation*}
\ln [S(b) / S(0)]=-b D_{a p p}+\frac{1}{6} b^{2} D_{a p p}^{2} K_{a p p} \tag{1}
\end{equation*}
$$

where $K_{\text {app }}$ is the apparent kurtosis coefficient (AKC) at a specific direction $x=$ $\left(x_{1}, x_{2}, x_{3}\right)^{T} \in \mathcal{S}^{2}$ (the unit sphere in $\Re^{3}$ ), which is defined by

$$
\begin{equation*}
K_{a p p}:=\frac{M_{D}^{2}}{D_{a p p}^{2}} W x^{4} \tag{2}
\end{equation*}
$$

with

$$
\begin{align*}
D_{\text {app }} & :=D x^{2}:=\sum_{i, j=1}^{3} D_{i j} x_{i} x_{j} \\
M_{D} & :=\frac{D_{11}+D_{22}+D_{33}}{3} ;  \tag{3}\\
W x^{4} & :=\sum_{i, j, k, l=1}^{3} W_{i j k l} x_{i} x_{j} x_{k} x_{l}
\end{align*}
$$

$D_{\text {app }}$ is known as apparent diffusion coefficient (ADC), $M_{D}$ as the mean ADC and $b$ as the $b$-value which has the following relationship:

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

here $g$ is the gradient strength, $\gamma$ is the proton gyromagnetic ratio, $\delta$ is a pulse duration, $\Delta$ is a time interval between the centres of the diffusion sensitizing gradient pulse. In diffusion imaging, the diffusion tensor $D$ should be restricted to have positive eigenvalues [1, 3, 11. This is due to the fact that the process of diffusion is physically not defined for the negative domain. Actually, $D$ is related to the covariance matrix of the diffusion displacement probability, which must be positive definite.

Equation (1) was derived in 12 as the core model of DKI to estimate $D_{\text {app }}$ and $K_{\text {app }}$ through measured $\ln [S(b) / S(0)]$. Mathematically, the right-hand side of (11) is an approximation (up to the fourth-order) of $\ln [S(b) / S(0)]$ viewed as a function of $b$. Note that odd orders are zero in this situation. On the other hand, the core model for DTI, corresponding to (11) after removing the term $\frac{1}{6} b^{2} D_{a p p}^{2} K_{a p p}$, is a secondorder approximation. Hence, in the aspect of mathematics, the model of DKI is
nothing but a try to detect information from the residual of the approximation by DTI. Nevertheless, the link between the fourth-order approximation term and the apparent diffusion kurtosis $K_{a p p}$ is one of the celebrated contributions in [12.

Once the imaging model is represented in mathematical language, there are mathematical rules. That is to say, there are preconditions for the "equality" of $\ln [S(b) / S(0)]$ and its approximation as stated in (1). The major precondition is: there is a range of $b$-values for the model (11) to make sense. Without loss of generality, we denote by this range as $\left[0, b_{\max }\right]$, since only nonnegative $b$-values are used in DKI. Intuitively speaking, the range $\left[0, b_{\max }\right]$ is one's Trust Region for the model (11).

After determining the trust region, we can get that when $b \in\left[0, b_{\max }\right]$, the right-hand side of (1) approximates $\ln [S(b) / S(0)]$ well. Due to the signal attenuation, $\ln [S(b) / S(0)]<0$ for any $b>0$, especially for $b \in\left(0, b_{\max }\right]$. So, $b D_{\text {app }}-\frac{1}{6} b^{2} D_{a p p}^{2} K_{a p p}>0$ for $b \in\left(0, b_{\max }\right]$ in view of model (11). However, how to guarantee this is a difficult issue in DKI. To our best knowledge, this issue has not been covered yet. Similar to DTI and its extensions [1, 3, 11, 23, we formally name such a problem as the positive definiteness of DKI. Actually, the positive definiteness for diffusion imaging has a long history and is of great importance, which is essential for the model to make sense physically [1, 3, 11, 13, 17]. Actually, in [13], a stronger requirement was imposed, i.e., the derivative of $b D_{a p p}-\frac{1}{6} b^{2} D_{a p p}^{2} K_{a p p}$ with respect to $b$ is positive.

For the convenience of the sequel analysis, we give an explicit statement here.
Problem 1. The positive definiteness of DKI means: for any $b$-value $b \in\left(0, b_{\text {max }}\right]$,

$$
b D x^{2}-\frac{1}{6} b^{2}\left(M_{D}\right)^{2} W x^{4}>0
$$

holds for any $x \in \mathcal{S}^{2}$.
Since $b \in\left(0, b_{\max }\right]$, Problem 1 means

$$
D x^{2}-\frac{1}{6} b\left(M_{D}\right)^{2} W x^{4}>0
$$

for any $x \in \mathcal{S}^{2}$ and $b \in\left(0, b_{\text {max }}\right]$. To guarantee this, it is sufficient to make sure

$$
\begin{equation*}
D x^{2}-\frac{1}{6} b_{\max }\left(M_{D}\right)^{2} W x^{4}>0 \tag{4}
\end{equation*}
$$

for any $x \in \mathcal{S}^{2}$, since $D$ is positive definite. Hence, the positive definiteness of DKI (Problem (1) is completely characterized by (4).
1.1. Notation. For the convenience of the sequel analysis, here we give some notation. Let $p \in \Re[x]$ be a polynomial in the indeterminate $x$ taking value in $\Re^{m}$, then $p$ is called positive definite (positive semidefinite, respectively) if $p(x)>0$ for all $x \in \Re^{m} \backslash\{0\}\left(p(x) \geq 0\right.$ for all $x \in \Re^{m}$, respectively). If $p$ is homogeneous, then $p$ is positive definite (positive semidefinite, respectively) if and only if $p(x)>0$ for all $x \in \mathcal{S}^{m-1}\left(p(x) \geq 0\right.$ for all $x \in \mathcal{S}^{m-1}$, respectively). Here $\mathcal{S}^{m-1}$ is the unit sphere in the $m$-dimensional standard Euclidean space.

For every supersymmetric tensor $T$ of order $n$ and dimension $m$, we associate it with a polynomial $p \in \Re[x]$ uniquely. Namely, $p(x):=\sum_{i_{1}, \ldots, i_{n}=1}^{m} T_{i_{1} \ldots i_{n}} x_{i_{1}} \cdots x_{i_{n}}$ for any $x \in \Re^{m}$. Conversely, given a homogeneous polynomial $p \in \Re[x]$, we could uniquely determine a supersymmetric tensor $T$ such that the polynomial associates to $T$ is $p$. Thus, $T$ is called positive definite (positive semidefinite, respectively) if $p$ is
positive definite (positive semidefinite, respectively). We will denote by $T \succ \mathbf{0}$ ( $T \succeq$ $\mathbf{0}$, respectively) if $T$ is positive definite (positive semidefinite, respectively). Similar to those in (3), we abbreviate $\sum_{i_{1}, \ldots, i_{n}=1}^{m} T_{i_{1} \ldots i_{n}} x_{i_{1}} \cdots x_{i_{n}}$ as $T x^{n}$ for convenience. Now, for any two tensors $T$ and $S$ of the same size, say order $n$ and dimension $m$, the inner product of $T$ and $S$ is defined as $T \bullet S:=\sum_{i_{1}, \ldots, i_{n}=1}^{m} T_{i_{1} \ldots i_{n}} S_{i_{1} \ldots, i_{n}}$. For any two tensors $S$ and $T$ of the same dimension, say $m$, and order $k$ and order $n$, respectively, we define the tensor product $S \otimes T$ of $S$ and $T$ as the supersymmetric tensor uniquely determined by the polynomial $\left(S x^{k}\right)\left(T x^{n}\right)$. For three tensors $S, T$, and $R$ of appropriate sizes, we use $S \otimes T \otimes R$ to denote $(S \otimes T) \otimes R$.
1.2. Optimization Problem. In this subsection, we describe the positive definiteness of DKI in more detail associated with the practical computation during imaging postprocess.

The above mentioned positive definite problem of DKI comes from the parameters estimation in imaging postprocess. The strategy for Diffusion Kurtosis Imaging process is: divide the imaging body into serval slices, and partition every slice into many voxels. $m$ gradient diffusion directions $\left\{g^{(j)} \in \mathcal{S}^{2} \mid j=1, \ldots, m\right\}$ are chosen. On every direction, serval, say $k+1, b$-values $\left\{b_{0}, b_{1}, \ldots, b_{k}\right\}$ are taken. Now, take the numerical postprocess for one voxel as an example. For every direction, we record the (average) signal $S\left(b_{i}\right)$ for the imaging of the $i$-th $b$-value.

So, we have $k+1$ signal $S\left(b_{i}\right)$ (including $S(0)$ usually, so let $b_{0}=0$ without loss of generality) for every direction. The following is the traditional method to estimate diffusion tensor $D$ and diffusion kurtosis tensor $W$ :

Step 1 For every direction, estimate $D_{a p p}$ and $K_{a p p}$ for that direction using (1) and the $k$ signal $S\left(b_{i}\right)$ for that direction. Namely, find $D_{\text {app }}$ and $K_{a p p}$ through the following nonlinear equations:

$$
\left\{\begin{array}{rc}
0 & =-\ln \left[S\left(b_{1}\right) / S(0)\right]-b_{1} D_{a p p}+\frac{1}{6} b_{1}^{2} D_{a p p}^{2} K_{a p p}  \tag{5}\\
& \vdots \\
0 & =-\ln \left[S\left(b_{k}\right) / S(0)\right]-b_{k} D_{a p p}+\frac{1}{6} b_{k}^{2} D_{a p p}^{2} K_{a p p}
\end{array}\right.
$$

Here $b_{i}$ for $i=1, \ldots, k$ are the $k$ nonzero $b$-values in the experiment. There are two variables $D_{\text {app }}$ and $K_{a p p}$ in the above nonlinear equations (5). Theoretically, a solution of (1.5) can be decided for $\mathrm{k}=2$. However, there exist random errors, systematical errors and so on. Hence, we need more than 2 nonzero $b$-values in general to get a least square solution. Actually, the following minimization problem is solved instead of (5):

$$
\begin{array}{cl}
\min & \|y\|_{2}  \tag{6}\\
\mathrm{s.t.} & y_{i}=-\ln \left[S\left(b_{i}\right) / S(0)\right]-b_{i} D_{a p p}+\frac{1}{6} b_{i}^{2} D_{a p p}^{2} K_{a p p}, \quad i=1, \ldots, k .
\end{array}
$$

Step 2 Then, estimate diffusion tensor $D$ from the $m$ estimated $D_{a p p}$ 's and diffusion kurtosis tensor $W$ from the $m$ estimated $K_{a p p}$ 's, respectively. We first form a vector $z^{(1)}$ with its $i$-th element being the $i$-th estimated $D_{\text {app }}$. Then, solve the following equations to get diffusion tensor $D$ :

$$
\left\{\begin{aligned}
z_{1}^{(1)} & =D\left(g^{(1)}\right)^{2} \\
& \vdots \\
z_{m}^{(1)} & =D\left(g^{(m)}\right)^{2}
\end{aligned}\right.
$$

Similarly, using $D$, the estimated $D_{a p p}, K_{a p p}$, (22) and (3), we can get a vector $z^{(2)}$ and the following equations for $W$ :

$$
\left\{\begin{aligned}
z_{1}^{(2)} & =W\left(g^{(1)}\right)^{4} \\
& \vdots \\
z_{m}^{(2)} & =W\left(g^{(m)}\right)^{4}
\end{aligned}\right.
$$

Since $W$ is supersymmetric in DKI, there are 15 independent variables in $W$. So, at least 15 non-collinear directions, i.e., $m \geq 15$, are needed to estimate $W$.

Similar to Step 1, we use two minimization problems instead of the above linear systems to get least square solutions:

$$
\begin{align*}
\min & \|y\|_{2} \\
\text { s.t. } & y_{i}=z_{i}^{(1)}-D\left(g^{(i)}\right)^{2}, \quad i=1, \ldots, m \tag{7}
\end{align*}
$$

and

$$
\begin{array}{cl}
\min & \|y\|_{2} \\
\text { s.t. } & y_{i}=z_{i}^{(2)}-W\left(g^{(i)}\right)^{4}, \quad i=1, \ldots, m . \tag{8}
\end{array}
$$

Obviously, the traditional procedure consisting of Step 1 and Step 2 does not guarantee the positive definiteness of DKI (Problem (1) theoretically. Now, with $t$ being an auxiliary variable, we propose our optimization model which serves as a suggestion for solving Problem 1 .

$$
\begin{array}{ll}
\min & t \\
\text { s.t. } & y_{(i-1) m+j}=-\ln \left[S\left(b_{i}\right) / S(0)\right]-b_{i} D \bullet g^{(j)}\left(g^{(j)}\right)^{T} \\
& \quad+\frac{1}{6} b_{i}^{2} \frac{\left(D_{11}+D_{22}+D_{33}\right)^{2}}{9} W \bullet\left(g^{(j)} \otimes g^{(j)} \otimes g^{(j)} \otimes g^{(j)}\right), \\
& \quad i=1, \ldots, k, \quad j=1, \ldots, m, \\
& (t, y) \in \mathcal{L}_{k m+1}, \\
& D \succ \mathbf{0}, \\
& \frac{6}{b_{\max }} I \otimes D-\frac{\left(D_{11}+D_{22}+D_{33}\right)^{2}}{9} W \succ \mathbf{0} .
\end{array}
$$

Here $\mathcal{L}_{k m+1}:=\left\{(t, y) \in \Re \times \Re^{k m} \mid t \geq\|y\|_{2}\right\}$ is a second order cone with size $k m+1$. Note that (9) is a nonlinear conic minimization problem in general. Here we state the main theoretical result.

Theorem 1.1. The solution of (9) satisfies the positive definiteness property in Problem 1.
Proof. Since $D \succ \mathbf{0}$, we get that $D x^{2}>0$ for any $x \in \mathcal{S}^{2}$. Note that

$$
\frac{6}{b_{\max }} I \bigotimes D-\frac{\left(D_{11}+D_{22}+D_{33}\right)^{2}}{9} W \succ \mathbf{0}
$$

means

$$
\begin{aligned}
0 & <\left(\frac{6}{b_{\max }} I \bigotimes D-\frac{\left(D_{11}+D_{22}+D_{33}\right)^{2}}{9} W\right) \bullet(x \bigotimes x \bigotimes x \bigotimes x) \\
& =\frac{6}{b_{\max }}(I \bullet x \bigotimes x)(D \bullet x \bigotimes x)-\left(M_{D}\right)^{2} W x^{4} \\
& =\frac{6}{b_{\max }} D x^{2}-\left(M_{D}\right)^{2} W x^{4}
\end{aligned}
$$

for any $x \in \mathcal{S}^{2}$. Here, the first equality follows from the definitions of $M_{D}$ and $W x^{4}$ (3), and the last from the definition of $D x^{2}$ (3) and $x \in \mathcal{S}^{2}$.

Remark 1. At the end of this section, we give some remarks on the minimization problem (9) and those in Step 1 and Step 2.

- We note that minimization problem (9) without the last two positive definiteness constraints is exactly a combination of minimization problems (6), (7) and (8). That is to say, we can combine Step 1 and Step 2 in the above discussion into one minimization problem. Such a combination will result in better approximation, i.e., the estimated $D$ and $W$ can fit the measured signal in view of (11) better. Nevertheless, the combined minimization problem is a nonlinear optimization problem with size larger than (6), (7) and (8).
- Comparing with (6) (an unconstrained nonlinear least square problem), (7) and (18) (two unconstrained linear least square problems), numerical methods for (9) (even without the positive definiteness constraints) are less efficient and robust. Hence, people likes to use Step 1 and Step 2 above instead of (9). However, (9) has two advantages: (i) it can provide a positive definite diffusion tensor $D$ which is of fundamental necessary [1, 3, 11, 23, while Step 1 and Step 2 above cannot guarantee this theoretically; (ii) it solves Problem 1 as well, which is essential for DKI as discussed above.
- In the next section, we will derive fast numerical solution method for (19).


## 2. Theory and Method

In this section, we discuss practical numerical solution methods for Problem 1. At first, we consider the numerical method for (9). Note that minimization problem (9) is a nonlinear conic optimization problem which is already hard to handle. Moreover, the last positive definite tensor conic constraint in (9) makes it intractable apparently [22]. However, the special fourth order three-dimensional property of $W$ gives an exception. At first, we prove the following result.

Theorem 2.1. Minimization problem (19) can be transformed into the following linear conic minimization problem:

$$
\begin{array}{cl}
\min & t \\
s . t . & y_{(i-1) m+j}= \\
& -\ln \left[S\left(b_{i}\right) / S(0)\right]-b_{i} D \bullet g^{(j)}\left(g^{(j)}\right)^{T} \\
& \quad+\frac{1}{6} b_{i}^{2} K \bullet\left(g^{(j)} \otimes g^{(j)} \otimes g^{(j)} \otimes g^{(j)}\right),  \tag{10}\\
& i=1, \ldots, k, j=1, \ldots, m, \\
& (t, y) \in \mathcal{L}_{k m+1}, \\
& D \succ \mathbf{0}, \\
& \frac{6}{b_{\text {max }}} I \otimes D-K \succ \mathbf{0} .
\end{array}
$$

Proof. Denote by the feasible solution set of (9) as $\mathcal{F}_{1}$ and that of (10) as $\mathcal{F}_{2}$. Then, for any $(t, y, D, W) \in \mathcal{F}_{1}$, we have $\left(t, y, D,\left(M_{D}\right)^{2} W\right) \in \mathcal{F}_{2}$; and conversely, for any $(t, y, D, K) \in \mathcal{F}_{2}$, we have $\left(t, y, D, \frac{K}{\left(M_{D}\right)^{2}}\right) \in \mathcal{F}_{1}\left(M_{D}>0\right.$ since $\left.D \succ \mathbf{0}\right)$. Note that the objective functions of both (9) and (10) are $t$. Hence, the optimal values of (9) and (10) are equal, since the projects of their feasible solution sets on the variable $t$ are the same. Moreover, we can derive an optimal solution of one from an optimal solution of the other in view of the above relation. The proof is complete.

Now, compared with the models which have sophisticated optimization softwares SeDuMi and SDPT3 [26, 27], the only difficulty in (10) is the last positive definite tensor conic constraint. Nevertheless, the following lemma provides a solution for this problem.

Lemma 2.2. Every positive semidefinite (hence, positive definite) real ternary quartic is a sum of at most six squares of quadratic forms.

Proof. From [7. Theorem 2.3], we know that every positive semidefinite real ternary quartic $p$ have a positive semidefinite matrix representation in the power vector $g:=\left(x_{1}^{2}, x_{1} x_{2}, x_{1} x_{3}, x_{2}^{2}, x_{2} x_{3}, x_{3}^{2}\right)^{T}$ [7, Pages 2-4]. That is to say that there exists a positive semidefinite matrix $M \in S^{6 \times 6}$ such that $p(x)=g^{T} M g$, here $S^{k \times k}$ means the $k \times k$ symmetric matrix space for a positive integer $k$. A direct decomposition for positive semidefinite matrix will yield the desired result. The proof is complete.

Now, using Lemma 2.2 and the fact that the cone of positive symmetric matrices is solid, we can derive an equivalent linear conic minimization problem from (10) with only positive definite matrix cone (positive tensor cone of order two [22]) and second order cone constraints.

$$
\begin{array}{cl}
\min & t \\
\text { s.t. } & y_{(i-1) m+j}=-\ln \left[S\left(b_{i}\right) / S(0)\right]-b_{i} D \bullet g^{(j)}\left(g^{(j)}\right)^{T} \\
& \quad+\frac{1}{6} b_{i}^{2} K \bullet\left(g^{(j)} \otimes g^{(j)} \otimes g^{(j)} \otimes g^{(j)}\right), \\
& \quad i=1, \ldots, k, j=1, \ldots, m,  \tag{11}\\
& \mathcal{P}(S)=\frac{6}{b_{\max }} I \otimes D-K, \\
& (t, y) \in \mathcal{L}_{k m+1}, \\
& D \succ \mathbf{0}, S \succ \mathbf{0} .
\end{array}
$$

Here $\mathcal{P}$ is a linear operator which maps a $6 \times 6$ symmetric matrix $S$ into a fourthorder three-dimensional supersymmetric tensor $T$ such that the polynomials are equal: $\left(x_{1}^{2}, x_{2}^{2}, x_{3}^{2}, x_{1} x_{2}, x_{1} x_{3}, x_{2} x_{3}\right) S\left(x_{1}^{2}, x_{2}^{2}, x_{3}^{2}, x_{1} x_{2}, x_{1} x_{3}, x_{2} x_{3}\right)^{T}=T x^{4}$ for any $x \in \Re^{3}$. In the following remark, we give an explicit formula of this linear operator.

Remark 2. We note that a fourth-order three-dimensional supersymmetric tensor $T$ has only 15 independent elements [21, 22]; while a symmetric matrix $S$ has 21 independent elements. However, we could uniquely determine the supersymmetric tensor $T$ from $S$ by the following formula [3]:

$$
\left.S=\begin{array}{cccccc}
H_{4,0,0} & 0 & 0 & \frac{1}{2} H_{3,1,0} & \frac{1}{2} H_{3,0,1} & 0  \tag{12}\\
0 & H_{0,4,0} & 0 & \frac{1}{2} H_{1,3,0} & 0 & \frac{1}{2} H_{0,3,1} \\
0 & 0 & H_{0,0,4} & 0 & \frac{1}{2} H_{1,0,3} & \frac{1}{2} H_{0,1,3} \\
\frac{1}{2} H_{3,1,0} & \frac{1}{2} H_{1,3,0} & y_{6} & H_{2,2,0} & \frac{1}{2} H_{2,1,1} & \frac{1}{2} H_{1,2,1} \\
\frac{1}{2} H_{3,0,1} & 0 & \frac{1}{2} H_{1,0,3} & \frac{1}{2} H_{2,1,1} & H_{2,0,2} & \frac{1}{2} H_{1,1,2} \\
0 & \frac{1}{2} H_{0,3,1} & \frac{1}{2} H_{0,1,3} & \frac{1}{2} H_{1,2,1} & \frac{1}{2} H_{1,1,2} & H_{0,2,2}
\end{array}\right]
$$

where $y_{i}$ are free parameters for all $i \in\{1,2, \ldots, 6\}$, and $H_{i, j, k}$ are coefficients of the following representation of $T x^{4}$ :

$$
T x^{4}:=\sum_{i+j+k=4} H_{i, j, k}\left(x_{1}\right)^{i}\left(x_{2}\right)^{j}\left(x_{3}\right)^{k}
$$

Hence, we can easily give the operator $\mathcal{P}$ in view of (12).

Remark 3. We note that although minimization problem (11) is equivalent to (10) in theoretical, the practical computation of (11) will be unstable, since variables $D$ and $K$ are not in the same order of magnitude, and variable $S$ is in small order of magnitude. In practical computation, $D$ is of order $O\left(10^{-3}\right)$ while $W$ is of order $O(1)$. Hence, $K$ and $S$ are of order $O\left(10^{-6}\right)$. So, we should scale $K$ and $S$ to get stable numerical results. For example, replacing $K$ and $S$ in (11) by $\frac{K}{b_{\max }}$ and $\frac{S}{b_{\max }}$, respectively, is a good choice.

Through the above analysis, we did not touch the method to decide $b_{\max }$. In general, the determination of $b_{\max }$ is as hard as the estimation problem (9) itself. Here we give two heuristic methods to determine $b_{\max }$ for the considered voxel:

- We can first use Step 1 and Step 2 to estimate diffusion tensor $D$ and diffusion kurtosis tensor $W$, then we use $D$ and $W$ to compute the largest $\left(D_{\text {app }} K_{\text {app }}\right)^{*}:=\max \left\{D_{\text {app }} K_{\text {app }} \mid x \in \mathcal{S}^{2}\right\}$, and finally set $b_{\text {max }}:=\frac{6}{\left(D_{\text {app }} K_{a p p}\right)^{*}}$. We can use some discrete method to get the largest $\left(D_{\text {app }} K_{\text {app }}\right)^{*}$. We note that a stronger relation was obtained in [13, Inequality (A2)] as $b_{\max } \leq$ $\frac{3}{\left(D_{\text {app }} K_{\text {app }}\right)^{*}}$, which is a consequence of a stronger condition than that in Prob$\operatorname{lem} 1$.
- We can just take simply the largest $b$-value we experimented, since the $b$ values we conducted are of course in our Trust Region. However, this method is feasible only for moderate $b$-values (e.g., $2000 \mathrm{~s} / \mathrm{mm}^{2}$ to $3000 \mathrm{~s} / \mathrm{mm}^{2}$ ), since the method is conservative when the tested $b$-value is too large.
Now, we can use sophisticated optimization softwares to solve minimization problem (11). For example, SeDuMi [26] and SDPT3 [27] can be employed to solve it. Till now, we complete the theoretical analysis as well as the practical methodology for Problem 1. For the convenience of reference, we denote by the above method as Conic.
2.1. Comparisons. In view of the proof in Theorem 2.1. we give some observations on the relationships between serval generalizations of DTI.

Remark 4. Using the idea in the proof of Theorem 2.1, we can restate the model (11) with (2) and (3) as

$$
\begin{equation*}
\ln [S(b) / S(0)]=-b D x^{2}+\frac{1}{6} b^{2} K x^{4} \tag{13}
\end{equation*}
$$

for the diffusion tensor $D$ and the fourth-order tensor $K$. Here $\frac{K}{\left(M_{D}\right)^{2}}$ is actually the diffusion kurtosis tensor $W$ in (3).

While the HOT model (here we only consider the real case up to fourth-order) in [14, Equation (25)] has the following form:

$$
\begin{equation*}
\ln [S(b) / S(0)]=-b^{(2)} D^{(2)} x^{2}+b^{(4)} D^{(4)} x^{4} \tag{14}
\end{equation*}
$$

where

$$
b^{(2)}=\gamma^{2} g^{2} \delta^{2}\left(\Delta-\frac{\delta}{3}\right) \text { and } b^{(4)}=\gamma^{4} g^{4} \delta^{4}\left(\Delta-\frac{3 \delta}{5}\right)
$$

and $D^{(2)}$ and $D^{(4)}$ are a second-order and a fourth-order tensors, respectively.
The fourth-order generalized DTI (GDTI) considered in [3, 18, 23, has the following form:

$$
\begin{equation*}
\ln [S(b) / S(0)]=-b H x^{4} \tag{15}
\end{equation*}
$$

for a fourth-order tensor $H$.

From (13), (14) and (15), we have:

- First, $b^{(2)}=b$. Then, since $\delta$ and $\Delta$ are known constants during imaging, we can get that $b^{(4)}=\kappa b^{2}$ for a positive constant $\kappa$. Absorbing this constant $\kappa$ into tensor $D^{(4)}$, (14) now is essential (13). Hence, DKI proposed in [12] is a special case of HOT proposed in [14] in this sense.
- Like HOT, (15) has higher order generalization [18, 23]. Nevertheless, it is hard to point out the relationship between GDTI and HOT (hence, DKI), since the right-hand side of (15) is always linear in $b$ while that of (14) is always nonlinear in $b$.

In the following, we compare our conic method Conic with existing methods for dealing with positive definiteness in diffusion imaging.

- When letting $K_{a p p} \equiv 0$ in (11), we arrive at DTI model. There is discussion on positive definiteness for DTI in the literature, see for example, [1]. The method in [1] is: parameterize diffusion tensor $D$ as its eigenvalues $\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right)$ and Euler-angles $\left(\alpha_{1}, \alpha_{2}, \alpha_{3}\right)$; restrict the eigenvalues $\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right)$ in a reasonable range, say $\left(10^{-7}, 10^{-2}\right)$, to ensure the positive definiteness of $D$; and, use some nonlinear optimization method, say sequential quadratic programming (SQP), to solve the resulting constrained nonlinear optimization problem. Please see [1. Pages 123-124] for a comprehensive reference.
- For the fourth-order GDTI model (15) considered in 3, they first use Lemma 2.2 to convert the corresponding optimization problem into a minimization problem involving positive semidefiniteness constraint like that in (9). Then, they employ a matrix decomposition technique to handle the positive semidefiniteness constraint, hence the resulting minimization problem becomes a familiar nonlinear minimization problem. By the way, a Riemannian framework which is similar to our positive definiteness constraint formula for (15) was proposed in [11. Nevertheless, they use general nonlinear optimization methods to solve their minimization problems. Please see [3, Pages 310-313] and [11, Page 860] for comprehensive references.
- For general GDTI considered in [23], they use the space tensor conic formula [22]. They also use a nonlinear optimization method to solve it.
- Our minimization problem (11) is a linear minimization problem under conic constraints. Unlike general nonlinear formulae in [1, 3, 11, 23, (11) can be solved in polynomial-time [26, 27]. Compared to the parameterization methods in [1, 3, the conic constraints in (11) have more simpler representations. Moreover, the resulting minimization problem (11) is linear. To our best knowledge, not only the conic formula but also the solution method suggested here are different from those in the literature.
2.2. A Simplified Practical Method. The theoretical analysis of Problem 1 results in a conic linear minimization problem (11). Although (11) is a linear optimization problem with simple formula, it is in the language of conic optimization. In this subsection, we give a simplified version of (11) in the language of familiar nonlinear programming which also presents another perspective to handle the positive definiteness of DKI (Problem (11)).

Besides that, there is another major factor that motivates us to consider a practical method for the traditional strategy, i.e., Step 1 and Step 2. When doing theoretical research, we can generate data set with as many $b$-values and directions as we want. Nevertheless, the data sets generated from hospitals for patients are
limited in view of the many $b$-values and directions. Take the situation in Tianjin First Central Hospital as an example, usually, 30 directions and two moderate $b$ values (e.g., $1000 \mathrm{~s} / \mathrm{mm}^{2}, 2000 \mathrm{~s} / \mathrm{mm}^{2}$ ) are allowed by the reality. The time needed for a scanner to get a data set around $70 \times 128 \times 128$ voxels of two $b$-values and 30 gradient directions for a patient's brain is around twenty minutes. Any longer time is unbearable for a patient. As we all know, such a data set is some kind of limitation to investigate DKI [12, 17]. At least, there should be serval $b$-values for estimating $D_{\text {app }}$ and $K_{a p p}$, see (6).

While, since conventional DTI is unable to handle non-Gaussian diffusion, how could we detect non-Gaussian diffusion from the above described data through DKI? This is just the problem Tianjin First Central Hospital faces to.

Putting aside Problem 1, when we use the traditional method (Step 1 and Step 2), 30 directions seem to be enough for the estimation problems (7) and (8), while only two nonzero $b$-values will result in unstable numerical computation for the nonlinear minimization (6). We note that: theoretically, two nonzero $b$-values together with $S(0)$ are enough for the nonlinear minimization (6), but the practical errors in data as well as the order of magnitude of $D_{\text {app }}$ being $O\left(10^{-3}\right)$ in general will result in unstable, even incorrect, numerical results.

Here, as a try to slove the above mentioned problems, we consider the following three minimization problems:

$$
\begin{align*}
\min & \|y\|_{2} \\
\text { s.t. } & y_{i}=-\ln \left[S\left(b_{i}\right) / S(0)\right]-b_{i} D_{a p p}+\frac{1}{6} b_{i}^{2} D_{a p p}^{2} K_{a p p}, \quad i=1, \ldots, k,  \tag{16}\\
& D_{\text {app }}>0, \\
& D_{\text {app }} K_{\text {app }} \leq \frac{6}{b_{\max }}, \\
& \min \quad\|y\|_{2} \\
& \text { s.t. } \quad y_{i}=z_{i}^{(1)}-D\left(g^{(i)}\right)^{2}, \quad i=1, \ldots, m, \\
& D \succ \mathbf{0},
\end{align*}
$$

and minimization problem (8).
Comparing with (6) and (7) in Step 1 and Step 2, we add more constraints into (16) and (17), respectively. Intuitively, constraint $D \succ 0$ in (17) is for the purpose of guaranteeing the positive definiteness of diffusion tensor $D$, and the two inequality constraints in (16) is for Problem (1) Note that (17) can be casted into the following linear problem:

$$
\begin{array}{cl}
\min & t \\
\mathrm{s.t.} & y_{i}=z_{i}^{(1)}-D\left(x^{(i)}\right)^{2}, \quad i=1, \ldots, m  \tag{18}\\
& D \succ \mathbf{0} \\
& (t, y) \in \mathcal{L}_{m+1}
\end{array}
$$

where $\mathcal{L}_{m+1}$ denotes a second order cone with size $m+1$. (18) can be efficiently solved through optimization softwares, say, SeDuMi and SDPT3. Obviously, (18) is different from the method in [1 for guaranteeing the positive definiteness of DTI.

Remark 5. As the practical data sets got in hospitals for patients have few $b$-values, typically $k=2$ (usually $k=1$ ), the resulting minimization problem (6) is of less robust. However, the additional constraints in (16) can narrow the feasible solution set of (6) largely while keep the theoretical optimal solution. Such a strategy can make minimization problem (16) more robust than (6). Hence, we are expected
to get more robust, also more exact (due to the positive definiteness) information, from (16) than that from (6).

Remark 6. We note that since we impose positive constraint for $D_{a p p}$ in (16), the positive definiteness constraint for matrix $D$ in (17) can be omitted in practice. In our implementation for the method in this subsection, we drop this positive definite constraint. We use it to test the real data set described in the next section. Nevertheless, only 283 voxels out of 5130 voxels where the computed $D$ is not positive definite if (16) is used for estimating $D_{a p p}$ and $K_{a p p}$.

We denote the practical method proposed in this subsection as PosDef for the convenience of reference in the sequel analysis.
2.3. Principal Parameters. In the numerical computation, we need some parameters of DKI. Of course, we put emphasis on the diffusion kurtosis tensor. We refer to [17, 12, 20, 21 for more parameters for DKI. Here we just discuss some principal parameters for illustration. In [21, based on the definition of D-eigenvalues of $W$, we can derive the mean kurtosis $M_{K}$ and the largest kurtosis $L_{K}$. D-eigenpair $(\lambda, x)$ means $\lambda \in \Re$ and $x \in \Re^{3}$ satisfying the following polynomial system:

$$
\left\{\begin{array}{l}
W x^{3}=\lambda D x  \tag{19}\\
D x^{2}=1
\end{array}\right.
$$

In [21, in order to find the D-eigenvalues, we must get the inverse $\bar{D}$ of $D$ first, then define a new fourth-order tensor $\bar{W}$ by $\bar{W}_{i j k l}:=\sum_{h=1}^{3} \bar{D}_{i h} W_{h j k l}$ (see 21, Equation (7) and Theorem 4] for more detail). The D-eigenvalues are calculated through $D$ and $\bar{W}$. We note that $W$ is of magnitude order of $O(1)$ in the practical computation, and $D$ is of order $O\left(10^{-3}\right)$. So, small error in $D$ can result in great disturbance in $\bar{D}$, hence in $\bar{W}$. Therefore, the computed $D$-eigenvalues are unstable in view of the practical computation in general. So, this, together with the limited source data sets in practice, can result in blur parameters maps based on $D$-eigenvalues.

Nevertheless, from the formula of $K_{a p p}$ in (2), we see that

$$
K_{a p p} D_{a p p}^{2}=M_{D}^{2} W x^{4}
$$

Hence the fourth-order term in (11) is $\frac{1}{6} b^{2} M_{D}^{2} W x^{4}=\frac{1}{6} b^{2} K x^{4}$, here $K$ is the tensor in (11). Since the difference of DTI and DKI is this term and it is completely characterized by tensor $K$, we can investigate the information provided by tensor $K$ instead. We think, of course, that the interest of DKI is on the tensor $K$. Now, similar to a matrix, consider $\lambda \in \Re$ and $x \in \Re^{3}$ satisfying the following system:

$$
\left\{\begin{array}{l}
K x^{3}=\lambda x  \tag{20}\\
x^{T} x=1
\end{array}\right.
$$

The above system (20) is the $Z$-eigenvalue problem proposed in [19]. The difference between (20) and (19) is that $\lambda$ computed through (20) is of the same order of magnitude of $K$ in general. Moreover, since $M_{D}$ is a constant once we got $D$. We can find the Z-eigenvalues of $W$ instead of that for $K$ :

$$
\left\{\begin{array}{l}
W x^{3}=\lambda x  \tag{21}\\
x^{T} x=1
\end{array}\right.
$$

Note that there is no effect of $D$ in (21) now, and the magnitude of $W$ is $O(1)$. So, we are expected to have a more stable numerical computation than that based on $D$-eigenvalues. At last, the expected Z-eigenvalues of $K$ are just $\left(M_{D}\right)^{2}$ times of those of $W$, see (20) and (21).

So, in this paper, we will investigate the parameter maps derived from the $Z$ eigenvalues of the tensor $K$. Especially, we will concentrate on the largest $Z$ eigenvalue and the mean of $Z$-eigenvalues. Here, we define the tensor $K$ for PosDef and the LS method (Step 1 and Step 2) just as the tensor $\left(M_{D}\right)^{2} W$. We note that the computed $Z$-eigenvalues of tensor $K$ are not the kurtosis, they are parameters for the fourth-order term in DKI, i.e., the additional information provided other than DTI.

## 3. Numerical Study

In this section, we report some numerical results based on both synthetical and real data for Conic, PosDef and the traditional LS method [12, 17] (see more details in Step 1 and Step 2, we abbreviate it as $\mathbf{L S}$ ). Since we consider data sets with only two nonzero b-values, a lower and upper bound for the indeterminate is added to $\mathbf{L S}$ to get reasonable $K_{\text {app }}$. All the numerical implementation are done on a PC with CPU of 3.4 GHz and RAM of 2.0 GB , and all codes are written in MATLAB. We use SDPT3 [27] to solve Conic (please see [27] for the method of formulating (11) into the required formula in SDPT3), while MATLAB Optimization Tools fmincon and lsqlin for constrained least square and unconstrained linear least square minimization problems in PosDef and LS. We use the method proposed in 21, Pages 153-155] to find all the Z-eigenvalues of the computed tensor $K$. Note that (20) is just the model discussed in [21] with $D=I$, the identity matrix.

Firstly, we present some numerical results on synthetical data. The synthetical data are generated by using the following multi-tensor model [9:

$$
S_{i}\left(b, g_{i}\right)=\sum_{k=1}^{n} \frac{1}{n} e^{-b D_{k} g_{i}^{2}}+\xi
$$

where $b$ is the $b$-value; $g_{i}$ is the $i$-th gradient direction for $i \in\{1,2, \ldots, N\} ; n \in$ $\{1,2,3,4\}$ is the number of fibers and $D_{1}:=[1390,355,355] \times 10^{-6} \mathrm{~mm}^{2} / \mathrm{s}$; while $D_{k}$ for $k \in\{2,3,4\}$ are generated by rotating $D_{1}$ with $\frac{\pi}{n}(k-1)$ in the x-y plane deasil, we see that $D_{k}$ is dependent on the chosen $n$ for individual experiment; and, $\xi$ is the Rician noise with standard deviation of $\frac{1}{\sigma}$, which produces an signal to noise ratio (SNR) of $\sigma$. In the numerical simulation, we choose $N=30$ and $b=1000,2000 \mathrm{~s} / \mathrm{mm}^{2}$.

We analyze the absolute error of the true logarithm signal and the estimated logarithm signal for four cases, i.e., with different $n$. The SNR varies from 5 to 50 . We simulate every case 100 times to get the mean absolute error. The numerical results are mapped in Figures 1-4.

From Figures 1-4, we find the followings:

- Although there are more constraints in (16) than those in (6), the estimation of (16) is not worse than that of (6). Note that, more constraints for an minimization problem will increase the optimal value in general, i.e., increase the error in our cases. Nevertheless, the well performance of PosDef in this test indicates that Problem 1 is essential for DKI. The results are similar for Conic.
- We note that Conic works better than both PosDef and LS when SNR is low. This coincides with the theoretical analysis: First note that Conic has more constraints than that of PosDef and LS. When SNR is low, the error between the estimated signal and the true signal is large, while the estimation methods compute $D$ and $W$ to fit the estimated signal. Hence, the fewer constraints in
the method, the better the computed $D$ and $W$ fitting the estimated signal, i.e., the worse the computed $D$ and $W$ fitting the true signal. When SNR is high, the error between the estimated signal and the true signal is small. Hence, the better the computed $D$ and $W$ fit the estimated signal, the better the computed $D$ and $W$ fit the true signal.
- The positive definiteness methods Conic and PosDef can provide a reasonable estimation for even complicated case we tested, i.e., $n=4$.
Secondly, we report some numerical results on a real data set. It is a human brain data set of $128 \times 128 \times 73$ voxels. The data set was acquired by a volunteer on a 3.0 T scanner at $b=0, b=1000 \mathrm{~s} / \mathrm{mm}^{2}$ and $b=2000 \mathrm{~s} / \mathrm{mm}^{2}$ with 30 encoding directions using a protocol approved by Tianjin First Central Hospital. In the following, we just list the numerical results of one slice (Slice 33) of the data set. We use $b_{\max }=2000 \mathrm{~s} / \mathrm{mm}^{2}$ throughout our computation.

We map some of the computational results in Figures 5-9. Figures 5-9 represent the ADC value of diffusion tensor $D$, the FA (Fractional Anisotropy) value of diffusion tensor $D$, the largest Z-eigenvalue of the tensor $K$, the mean of the Z-eigenvalues of the tensor $K$ and the largest AKC value (the largest D-eigenvalue of tensor $W$ ) computed by LS, PosDef and Conic (left to right), respectively.

All the above figures are just for some intuitive illustrations. It can be seen that Conic and PosDef can provide ADC and FA images similar to LS; and, the former gives slightly more clear images computed from the fourth-order tensor $K$ as well as the largest AKC value map than LS. Compared with Figure 5, Figure 7 represents some complementary information to the ADC map. Hence, these indicate that imposing Problem 1 into the analysis of DKI may provide us more useful information.

## 4. Conclusion

In this paper, we proposed a parameter estimation method (Conic) in DKI involving the positive definiteness. Such a method was analyzed both theoretically and practically. The preliminary numerical behavior of this method, its simplified version and that of the traditional LS method were compared on both synthetical and real data. We found that detecting positive definiteness of DKI has the potential to archive more useful information for us. An important aspect of the practical method discussed in this paper is that it was also designed to handle clinic data which is a "limited" data set compared to the data sets analyzed in the literature. There are a lot of issues, such as segmentation, registration and fiber tracking based on DKI using the methods proposed here. These are our future topics. Since GDTI and HOT are different in general, the positive definiteness of GDTI discussed in 23] cannot be transplanted to that of HOT directly. Hence, the positive definiteness of HOT is worth investigating. A stronger requirement than the positive definiteness of DKI was imposed in [13, Appendix], it would be interesting to extend the method in this paper to consider that.

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Figure 1. Comparisons of LS, PosDef and Conic on synthetic data with one fiber.

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Figure 2. Comparisons of LS, PosDef and Conic on synthetic data with two fibers.


Figure 3. Comparisons of LS, PosDef and Conic on synthetic data with three fibers.


Figure 4. Comparisons of LS, PosDef and Conic on synthetic data with four fibers.


Figure 5. ADC value map: LS, PosDef and Conic.


Figure 6. FA value map: LS, PosDef and Conic.


Figure 7. The largest Z-eigenvalue map: LS, PosDef and Conic.


Figure 8. The mean Z-eigenvalue map: LS, PosDef and Conic.


Figure 9. AKC value map: LS, PosDef and Conic.


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