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The direct tensor solution and higher-order acquisition schemes for generalized diffusion tensor imaging

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ABSTRACT

Both in diffusion tensor imaging (DTI) and in generalized diffusion tensor imaging (GDTI) the relation between the diffusion tensor and the measured apparent diffusion coefficients is given by a tensorial equation, which needs to be inverted in order to solve the diffusion tensor. The traditional way to do this does not preserve the tensorial structure of the equation, which we consider a weakness in the method.

For a physically correct measurement procedure, the condition number of the acquisition scheme, which is a determinant of the noise behavior, needs to be rotationally invariant. The method which traditionally is used to find such schemes, however, is cumbersome and mathematically unsatisfactory. This is considered a second weakness, closely connected to the first.

In this paper we present an alternative inversion of the diffusion tensor equation, which does preserve the tensor form, for arbitrary order, and which is named the *direct tensor solution* (*DTS*). The DTS is derived under the assumption that the apparent diffusion coefficient in any direction is known, i.e. in the *infinite* acquisition scheme.

Whenever the DTS is valid for a given *finite* acquisition scheme and for a given order, the condition number is rotationally invariant. The DTS provides a compact, algebraic procedure to check this rotational invariance. We also present a method to construct acquisition schemes, for which the DTS is valid for the measurement of higher-order diffusion tensors.

Furthermore, the DTS leads to other mathematical insights, such as tensorial relationships between diffusion tensors of different orders, and a more general understanding of the Platonic Variance Method, which we published before.

1. Introduction

Diffusion tensor imaging (DTI) [1] is an MRI technique that characterizes anisotropic diffusion in tissues. It is widely applied in the brain [2,3] and increasingly more in other tissues as well, like muscles [4] and kidneys [5,6]. Anisotropic diffusion is caused by the presence of collectively oriented cell structures, like the axons in white matter tracts, which allow a relatively easy random motion of the water molecules in one direction (along the axons), whereas the motion in other directions (perpendicularly to the axons) is more restricted.

Generalized diffusion tensor imaging (GDTI), introduced by Özarslan and Mareci [7], is an extension of DTI to address the *crossing fiber problem*, i.e. to describe the situation where more than one structural orientation is present in a voxel. Whereas DTI describes the diffusion with a second-order diffusion tensor, GDTI uses tensors of higher order. Especially the fourth-order diffusion tensor has already been used in a number of investigations [8–13].

Both DTI and GDTI use a diffusion weighted sequence to measure the apparent diffusion coefficient, A. The key part of such a sequence is the *diffusion weighting gradient* or *diffusion encoding gradient*. The timing and strength of this gradient determine the degree of diffusion weighting, b, and the direction of the gradient, $\mathbf{g}$, determines the direction in which the diffusion is measured. (For a more detailed treatment of a diffusion weighted sequence, see e.g. [3].) The relation between the MRI signal without diffusion weighting, S_0, and the signal with diffusion weighting, $S(b,\mathbf{g})$, is given by:

$$S(b,\mathbf{g}) = S_0 e^{-bA(\mathbf{g})}. \tag{1}$$

So when S_0 and $S(b,\mathbf{g})$ with chosen values of b and $\mathbf{g}$ are acquired, $A(\mathbf{g})$ can be calculated from Eq. (1). When the diffusion is isotropic, $A(\mathbf{g})$ has the same value in all directions and it is sufficient to measure in one direction only. In anisotropic tissues $A(\mathbf{g})$ has to be measured in a number of directions.

In DTI, the directional dependency of $A(\mathbf{g})$ is given by the relationship:

$$A(\mathbf{g}) = \sum_{i,j\in\{x,y,z\}} g_i g_j D_{ij}, \tag{2}$$

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where D_{ij} are the elements of the second-order *diffusion tensor*, and g_i and g_j are the components of the unit direction vector $\mathbf{g}$. In GDTI a generalization of Eq. (2) is used, with a tensor of order R:

$$A(\mathbf{g}) = \sum_{i_1 i_2 \cdots i_R \in \{x,y,z\}} g_{i_1} g_{i_2} \cdots g_{i_R} D_{i_1 i_2 \cdots i_R}, \tag{3}$$

Since the diffusion sequences which are used in practice always measure the same $A(\mathbf{g})$ value for $\mathbf{g}$ and $-\mathbf{g}$, one can only determine (generalized) diffusion tensors with even order, although theoretical models using odd-order tensors have been published [14]. Furthermore, Eq. (3) implies that the diffusion tensor is symmetric, i.e. its value does not change under permutations of the indices. The number of independent elements of a symmetric tensor of order R equals $M = (R+1)(R+2)/2$ [7], so in order to determine the diffusion tensor, $A(\mathbf{g})$ has to be measured in a number of directions $N \geqslant M$.

The set of measurement directions, $\{\mathbf{g}[1], \mathbf{g}[2], \ldots, \mathbf{g}[N]\}$, is called the *acquisition scheme* (also *encoding scheme* or *sampling scheme*). Calculating the diffusion tensor from the measured apparent diffusion coefficients, $A[n] = A(\mathbf{g}[n])$, requires inverting Eq. (3). Traditionally this is done using methods from linear algebra [1,3], which is possible since Eq. (3) establishes a linear relation between the $A[n]$ and the elements of D. To be able to apply linear algebra, however, a regrouping of Eq. (3) is necessary: the independent elements of D are put in a column, like a vector, D_m ($m = 1 \cdots M$), and Eq. (3) is rewritten into a matrix–vector equation: $A[n] = \sum_m G_{nm} D_m$. Using the (pseudo-)inverse of the matrix G one can calculate D_m.

This regrouping of a tensorial equation is the first of two fundamental weaknesses, or problems in the traditional way the (G)DTI experiment is conducted, that form the reason for this paper. Tensor equations have their own mathematical structure, properties, and algebraic rules that allow an efficient mathematical analysis. The central theme in tensor algebra is how equations behave under transformations of the co-ordinate frame. E.g. if one derives scalars following the rules of tensor algebra, these scalars always are rotationally invariant. Furthermore, tensor algebra gives rise to compact formulations which are particularly insightful. One of the major feats of tensor algebra is the theory of general relativity [15].

Regrouping the elements of a tensor equation, is like writing out all the components of a matrix equation, and trying to solve it brushing aside the instruments of matrix algebra. Obviously this is a contraproductive procedure: multiplying two rotations would become quite complicated; finding a general expression for the inversion of a set of linear equations would be practically impossible. Similarly we may be seriously wronging ourselves by disturbing the structure of a tensorial equation.

The second fundamental problem of (G)DTI is about acquisition schemes, and more precisely with the rotational invariance of the condition number. The condition number, κ, of an acquisition scheme characterizes the noise properties of the acquisition scheme, i.e. how the noise in the measurement data propagates to the results [8,16–18]; the smaller κ the better the noise properties. It is found in literature that the condition number of many acquisition schemes, which are used in practice, varies when the scheme is rotated [17,19]. Since κ depends only on the acquisition scheme (and not e.g. on the relative orientation of the tensor being measured), this is equivalent to the statement that κ varies with rotations of the co-ordinate frame, constituting an undesirable situation: rotations of the co-ordinate frame are purely mathematical and they should have no effect on any of the physical outcomes of an experiment. For a physically correct measurement, rotational invariance of κ is a prerequisite.

In the literature much attention has been paid to investigating acquisition schemes [e.g. 16–21] and schemes with an invariant κ have indeed been found. For a second-order tensor, these schemes appear to have icosahedral symmetry, and a κ of $\tfrac{1}{2}\sqrt{10}$ (≈ 1.58). For a fourth-order tensor, there is only one study which found a scheme with an almost invariant κ of 3.75 [8]. A problem remains, however: the procedure to find these schemes is rather cumbersome, it consists of simply trying a number of schemes, and each time checking the variation of κ under a large number of rotations. This is a time consuming procedure, it is never conclusive in a mathematical sense of the word, and it gives no insight in what constitutes a proper scheme.

Because of the nature of the two problems, one expects they are connected somehow, and therefore we formulate the following two questions to investigate in this paper: (1) *Does there exist a general expression for the inverse of* Eq. (3) *that preserves the tensor form?* (2) *Can we use this expression to formulate mathematical properties and a simple checking procedure for acquisition schemes with a rotationally invariant condition number?*

A general tensorial expression for the inverse of Eq. (3) should not depend on any particular acquisition scheme; when investigating this, we therefore assume that the apparent diffusion coefficient, A, is known in all directions. This is also known as the *infinite acquisition scheme*, which is, as [17] put it: "an ideal, albeit impractical, sampling scheme [involving] an infinite number of uniformly distributed directions, which would not privilege a specific set of orientations". We will show below, that under these conditions, the desired inverse expression of Eq. (3) can be derived for *arbitrary order*; we name it the *direct tensor solution* (DTS).

Next we investigate the conditions for which the DTS is valid for a finite acquisition scheme. There appears to be a relatively simple test for this, and we find that if the direct tensor solution is valid for a specific order, then κ is rotationally invariant. The maximum order for which the DTS is valid depends on the specific acquisition scheme, and is called *the order of the acquisition scheme*. We also present a method to *construct* higher-order acquisition schemes, by the introduction of weighting factors: a weighting factor in a way represents the solid angle covered by the individual measurement direction.

The DTS actually provides more opportunities to gain mathematical insight in (G)DTI. We show two more applications. The DTS leads to a natural way of defining relations between tensors of different orders. And finally, we investigate the consequences of the DTS to the Platonic Variance Method, which we published before [22].

A preliminary version of some of the results of this paper has been published as an e-poster at a meeting [23].

1.1. Definitions and conventions

We use $\boldsymbol{\omega}$ as a short notation for the spherical co-ordinates: $\boldsymbol{\omega} = (\vartheta, \varphi)$, $\vartheta = 0 \cdots \pi$ and $\varphi = 0 \cdots 2\pi$. $\mathbf{g}(\boldsymbol{\omega})$ is the unit vector in the direction $\boldsymbol{\omega}$; in Cartesian co-ordinates:

$$\mathbf{g}(\boldsymbol{\omega}) = \begin{pmatrix} \sin\vartheta\cos\varphi \\ \sin\vartheta\sin\varphi \\ \cos\vartheta \end{pmatrix}. \tag{4}$$

We use the following abbreviation to write the integral over the sphere:

$$\int_\Omega \cdots d\boldsymbol{\omega} = \int_0^{2\pi} \int_0^{\pi} \cdots \sin\vartheta \, d\vartheta \, d\varphi. \tag{5}$$

The operator SYM takes an arbitrary tensor F and turns it into a symmetric tensor E by averaging over all permutations of the indices, $P(i_1, i_2, \ldots, i_R)$:

$$E_{i_1 i_2 \cdots i_R} = \mathrm{SYM}\, F_{i_1 i_2 \cdots i_R} = \frac{1}{R!} \sum_{\substack{j_1 j_2 \cdots j_R \\ \in P(i_1 i_2 \cdots i_R)}} F_{j_1 j_2 \cdots j_R}. \tag{6}$$

When the SYM operator is meant to act only on certain indices, this is specified by subscripts underneath the SYM symbol.

The double factorial operator, !!, is defined as in [24]:

$$(2n+1)!! = 1 \cdot 3 \cdots (2n+1); \quad (-1)!! = 1; \\ (2n)!! = 2 \cdot 4 \cdots (2n); \quad 0!! = 1 \tag{7}$$

Two useful properties, which follow from Eq. (7), are:

$$n! = n!! \cdot (n-1)!!; \quad (2n)!! = n! \cdot 2^n \tag{8}$$

We chose not to use the more common notation for symmetrization, using parentheses around the indices: $F_{(i_1 i_2 \cdots i_R)}$ [25], since in the complex expressions we are going to deal with, this notation might soon become obscure. We did not adopt the Einstein summation convention either, since we will deal both with summations over co-ordinate indices, and with series summations. The Einstein convention applies only to the former, and using it would remove only part of the summation signs, which might have a confusing result.

2. The direct tensor solution

2.1. Summary

When diffusion is described by a diffusion tensor of order R, $D_{i_1 i_2 \cdots i_R}$, the apparent diffusion coefficient, $A(\boldsymbol{\omega})$, measured in the direction $\boldsymbol{\omega}$, is given by:

$$A(\boldsymbol{\omega}) = \sum_{\substack{i_1 i_2 \cdots i_R \\ \in\{x,y,z\}}} g_{i_1}(\boldsymbol{\omega}) g_{i_2}(\boldsymbol{\omega}) \cdots g_{i_R}(\boldsymbol{\omega}) D_{i_1 i_2 \cdots i_R}. \tag{9}$$

(Henceforward, in summations over co-ordinate indices the range $\{x, y, z\}$ is understood and is not written explicitly.) Using the infinite acquisition scheme, the inverse relationship we are looking for, i.e. the DTS, must be an expression which integrates over all directions (i.e. the sphere) and which is linear in $A(\boldsymbol{\omega})$:

$$D_{i_1 i_2 \cdots i_R} = \frac{1}{4\pi} \int_\Omega S_{i_1 i_2 \cdots i_R}(\boldsymbol{\omega}) A(\boldsymbol{\omega}) d\boldsymbol{\omega}. \tag{10}$$

(The factor $1/4\pi$ is used for convenience.) S is the *solution tensor*, which is required to depend on $\boldsymbol{\omega}$ only through $\mathbf{g}(\boldsymbol{\omega})$. The solution tensor may also contain Kronecker deltas, δ_{ij}, which play the role of constant tensors.

We postulate that S is constructed of $\mathbf{g}(\boldsymbol{\omega})$s and Kronecker deltas, using three basic operations: addition, tensor multiplication and multiplication with real numbers. Since $D_{i_1 i_2 \cdots i_R}$ is symmetric, tensor products of $\mathbf{g}(\boldsymbol{\omega})$s and Kronecker deltas have to be symmetric and they need to have the following form:

$$T^{(R,q)}_{i_1 i_2 \cdots i_R}(\boldsymbol{\omega}) = \mathrm{SYM}(g_{i_1}(\boldsymbol{\omega}) g_{i_2}(\boldsymbol{\omega}) \cdots g_{i_q}(\boldsymbol{\omega}) \delta_{i_{q+1} i_{q+2}} \cdots \delta_{i_{R-1} i_R}) \quad [q \text{ even}]. \tag{11}$$

Stated in words: $T^{(R,q)}$ consists of q components of $\mathbf{g}$, complemented with $(R-q)/2$ deltas to make a tensor of order R. The operator SYM guarantees that the result is symmetric. Our solution tensor then is a linear combination of these $T^{(R,q)}$:

$$S_{i_1 i_2 \cdots i_R}(\boldsymbol{\omega}) = \sum_{q=0,2,\ldots,R} \alpha(R,q) T^{(R,q)}_{i_1 i_2 \cdots i_R}(\boldsymbol{\omega}), \tag{12}$$

with coefficients $\alpha(R, q)$, which are undetermined, as yet.

If the solution tensor has the correct form, substitution of Eqs. (11), (12), and (9) into Eq. (10) will produce the identity. So the essential question is: do coefficients $\alpha(R, q)$ exist, for which this is the case? We shall demonstrate below that such coefficients indeed do exist, and that they are given by:

$$\alpha(R,q) = \frac{(R+q+1)!!}{(R-q)!!\,q!} (-1)^{\frac{R-q}{2}} \quad [q = 0, 2, \ldots, R]. \tag{13}$$

Fig. 1 shows the solution explicitly worked out for orders 0, 2, 4 and 6.

$$D = \frac{1}{4\pi} \int_\Omega A(\boldsymbol{\omega})\, d\boldsymbol{\omega}$$

$$D_{ij} = \frac{1}{4\pi} \int_\Omega \left(-\tfrac{3}{2}\delta_{ij} + \tfrac{15}{2} g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega}) \right) A(\boldsymbol{\omega})\, d\boldsymbol{\omega}$$

$$\begin{aligned} D_{ijkl} = \frac{1}{4\pi} \int_\Omega \Big(& \tfrac{15}{8}\mathrm{SYM}(\delta_{ij}\delta_{kl}) \\ & - \tfrac{105}{4}\mathrm{SYM}(g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega})\delta_{kl}) \\ & + \tfrac{315}{8} g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega}) g_k(\boldsymbol{\omega}) g_l(\boldsymbol{\omega}) \Big) A(\boldsymbol{\omega})\, d\boldsymbol{\omega} \end{aligned}$$

$$\begin{aligned} D_{ijklmn} = \frac{1}{4\pi} \int_\Omega \Big(& -\tfrac{35}{16}\mathrm{SYM}(\delta_{ij}\delta_{kl}\delta_{mn}) \\ & + \tfrac{945}{16}\mathrm{SYM}(g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega})\delta_{kl}\delta_{mn}) \\ & - \tfrac{3465}{16}\mathrm{SYM}(g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega}) g_k(\boldsymbol{\omega}) g_l(\boldsymbol{\omega})\delta_{mn}) \\ & + \tfrac{3003}{16} g_i(\boldsymbol{\omega}) g_j(\boldsymbol{\omega}) g_k(\boldsymbol{\omega}) g_l(\boldsymbol{\omega}) g_m(\boldsymbol{\omega}) g_n(\boldsymbol{\omega}) \Big) A(\boldsymbol{\omega})\, d\boldsymbol{\omega} \end{aligned}$$

Fig. 1. Direct tensor solutions for orders 0, 2, 4, and 6.

2.2. The H tensor equation

To deduce the coefficients $\alpha(R, q)$ we start with substituting Eqs. (11), (12), and (9) into Eq. (10):

$$\begin{aligned} D_{i_1 i_2 \cdots i_R} = \frac{1}{4\pi} \int_\Omega & \sum_{q=0,2,\ldots,R} \alpha(R,q) \\ & \times \mathrm{SYM}(g_{i_1}(\boldsymbol{\omega}) g_{i_2}(\boldsymbol{\omega}) \cdots g_{i_q}(\boldsymbol{\omega}) \delta_{i_{q+1} i_{q+2}} \cdots \delta_{i_{R-1} i_R}) \\ & \times \sum_{j_1 j_2 \cdots j_R} g_{j_1}(\boldsymbol{\omega}) g_{j_2}(\boldsymbol{\omega}) \cdots g_{j_R}(\boldsymbol{\omega}) D_{j_1 j_2 \cdots j_R}\, d\boldsymbol{\omega} \end{aligned} \tag{14}$$

Reordering such that the integral over $\boldsymbol{\omega}$ is moved inward as much as possible, and the summation over q is moved outward yields

$$\begin{aligned} D_{i_1 i_2 \cdots i_R} = \sum_{q=0,2,\ldots,R} \alpha(R,q) \underset{i_1 i_2 \cdots i_R}{\mathrm{SYM}} \Bigg(& \delta_{i_{q+1} i_{q+2}} \cdots \delta_{i_{R-1} i_R} \sum_{j_1 j_2 \cdots j_R} D_{j_1 j_2 \cdots j_R} \\ & \times \frac{1}{4\pi} \int_\Omega g_{j_1}(\boldsymbol{\omega}) g_{j_2}(\boldsymbol{\omega}) \cdots g_{j_R}(\boldsymbol{\omega}) g_{i_1}(\boldsymbol{\omega}) g_{i_2}(\boldsymbol{\omega}) \cdots g_{i_q}(\boldsymbol{\omega}) d\boldsymbol{\omega} \Bigg), \end{aligned} \tag{15}$$

where the subscripts under the SYM operator indicate that the operator acts on the i indices only, i.e. the SYM operation is executed after the summation over the j indices has been performed. The integrals in Eq. (15) have the form

$$H_{i_1 i_2 \cdots i_P} = \frac{1}{4\pi} \int_\Omega g_{i_1}(\boldsymbol{\omega}) g_{i_2}(\boldsymbol{\omega}) \cdots g_{i_P}(\boldsymbol{\omega}) d\boldsymbol{\omega}, \tag{16}$$

with $P = R, R+2, \ldots, 2R$. Let n_x, n_y, and n_z denote the number of occurrences of x, y, and z in $\{i_1, i_2, \ldots, i_R\}$, so $n_x + n_y + n_z = P$. By substituting the co-ordinates of $\mathbf{g}$ from Eq. (4) into Eq. (16) we are able to evaluate the integral, e.g. using a table of integrals [24]:

$$\begin{aligned} H_{i_1 i_2 \cdots i_P} &= \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (\sin\vartheta\cos\varphi)^{n_x} (\sin\vartheta\sin\varphi)^{n_y} (\cos\vartheta)^{n_z} \sin\vartheta\, d\vartheta\, d\varphi \\ & \begin{cases} = \dfrac{(n_x-1)!!(n_y-1)!!(n_z-1)!!}{(P+1)!!} & [n_x, n_y, \text{ and } n_z \text{ even}] \\ = 0 & [\text{otherwise}] \end{cases} \\ & \equiv H(n_x, n_y, n_z) \end{aligned} \tag{17}$$

The result is called the H function, $H(n_x, n_y, n_z)$.

A disadvantage of Eq. (17) is that it is a function of n_x, n_y, n_z instead of $i_1, i_2, \ldots, i_P$, so the tensor structure is lost. An expression in tensor form, which is needed in this context, is found by observing that the result of Eq. (17) is invariant under rotations of the coordinate system; this is in fact a natural consequence of the integration over the sphere. A tensor of which the individual elements are rotationally invariant is called an isotropic tensor [26]. One may construct an even-order symmetric isotropic tensor by symmetrizing a product of Kronecker deltas, which obeys the following relation:

$$\frac{1}{P+1}\mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4}\cdots\delta_{i_{P-1} i_P}) = H(n_x, n_y, n_z) \quad [P \text{ even}] \tag{18}$$

Eq. (18) is proven as follows. The SYM-operator expands to $P!$ terms with in each term a product of $P/2$ deltas, and each with a unique permutation of the indices $i_1, i_2, \ldots, i_P$. For a non-zero term, all deltas must yield 1, i.e. they must be of the form δ_{xx}, δ_{yy}, or δ_{zz}. It follows that for the existence of non-zero terms n_x, n_y, and n_z have to be even, otherwise the total result will be zero.

Given n_x, n_y, and n_z even, the terms with a non-zero contribution consist of $n_x/2$ deltas of the form δ_{xx}, $n_y/2$ deltas of the form δ_{yy}, and $n_z/2$ deltas of the form δ_{zz}. The number of ways to divide the $P/2$ deltas into three groups of sizes $n_x/2$, $n_y/2$, and $n_z/2$ is given by the multinomial distribution: $(P/2)!/((n_x/2)!\cdot(n_y/2)!\cdot(n_z/2)!)$. Distributing the indices over their deltas may be done in $n_x!\cdot n_y!\cdot n_z!$ ways. Some algebraic manipulation, using Eq. (8) shows that this amounts to a total of $P!!\cdot(n_x-1)!!\cdot(n_y-1)!!\cdot(n_z-1)!!$ permutations with a non-zero contribution. Dividing this by $P!$ (because of the SYM) and by $(P+1)$ (which is the factor before the SYM in Eq. (18)), the result of Eq. (17) is obtained.

Combining Eqs. (16)–(18) yields the *H tensor equation*:

$$\frac{1}{4\pi}\int_\Omega g_{i_1}(\boldsymbol{\omega})g_{i_2}(\boldsymbol{\omega})\cdots g_{i_P}(\boldsymbol{\omega})d\boldsymbol{\omega} = \frac{1}{P+1}\mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4}\cdots\delta_{i_{P-1} i_P}), \tag{19}$$

which will be used repeatedly throughout this paper. Fig. 2 shows examples of this equation, explicitly worked out for orders 2 and 4.

2.3. Further derivation

By substituting Eq. (19) into Eq. (15) we obtain:

$$D_{i_1 i_2\cdots i_R} = \sum_{q=0,2\cdots R}\alpha(R,q)\,\mathop{\mathrm{SYM}}_{i_1 i_2\cdots i_R}\left(\delta_{i_{q+1} i_{q+2}}\cdots\delta_{i_{R-1} i_R}\sum_{j_1 j_2\cdots j_R} D_{j_1 j_2\cdots j_R} \times\frac{1}{R+q+1}\mathrm{SYM}(\delta_{j_1 j_2}\cdots\delta_{j_{R-1} j_R}\delta_{i_1 i_2}\cdots\delta_{i_{q-1} i_q})\right) \tag{20}$$

The innermost SYM expression in Eq. (20) consists of $(R+q)!$ terms having $(R+q)/2$ deltas each. These deltas can be divided into three types. Firstly, deltas with one i and one j index; on summation over the j indices these deltas cause a *substitution* of a j index under the diffusion tensor by an i index. Secondly, deltas with two j indices; on summation over the j indices these deltas cause a *contraction* of the diffusion tensor (i.e. summing over two equal indices, which results in a tensor with an order lowered by 2). Thirdly, deltas with two i indices; summation over the j indices has no influence on them and they can be grouped with the deltas before the summation sign.

$$\frac{1}{4\pi}\int_\Omega g_i(\boldsymbol{\omega})g_j(\boldsymbol{\omega})\,d\boldsymbol{\omega} = \tfrac{1}{3}\delta_{ij}$$

$$\frac{1}{4\pi}\int_\Omega g_i(\boldsymbol{\omega})g_j(\boldsymbol{\omega})g_k(\boldsymbol{\omega})g_l(\boldsymbol{\omega})\,d\boldsymbol{\omega} = \tfrac{1}{5}\mathrm{SYM}(\delta_{ij}\delta_{kl}) = \tfrac{1}{15}\delta_{ij}\delta_{kl} + \tfrac{1}{15}\delta_{ik}\delta_{jl} + \tfrac{1}{15}\delta_{il}\delta_{jk}$$

Fig. 2. The H tensor equation for orders $P = 2$ and 4.

To count how many terms there are with exactly s deltas of the first type ($s \leqslant q$, s even) we first select from the total of $R/2 + q/2$ deltas three groups for the three types: this can be done in $(R/2+q/2)!/\{(R/2-s/2)!\cdot(q/2-s/2)!\cdot s!\}$ ways. We select s i indices, giving $q!/((q-s)!\cdot s!)$ ways, and s j indices: $R!/((R-s)!\cdot s!)$ ways. We distribute them over the selected deltas of the first type: the i indices give $s!$ ways, the j indices also $s!$ ways, and permutation of the i and j index on the same delta produces an other 2^s possibilities. The $R-s$ remaining j indices can be attached to the selected deltas of the second type in $(R-s)!$ ways, and likewise can the remaining i indices be attached to the deltas of the third type in $(q-s)!$ ways. Multiplying all these possibilities and developing this, we find a total of $(R+q)!!\cdot q!\cdot R!/\{(R-s)!!\cdot(q-s)!!\cdot s!\}$ terms. "Meta-mathematically" we write:

$$\mathrm{SYM}(\delta_{j_1 j_2}\cdots\delta_{j_{R-1} j_R}\delta_{i_1 i_2}\cdots\delta_{i_{q-1} i_q}) = \frac{1}{(R+q)!}\sum_{s=0,2,\cdots,q}\frac{(R+q)!!q!R!}{(R-s)!!(q-s)!!s!} \times\left\{\begin{array}{l} s \text{ deltas with one } i \text{ and one } j \text{ index} \\ \times(R/2-s/2) \text{ deltas with two } j \text{ indices} \\ \times(q/2-s/2) \text{ deltas with two } i \text{ indices}\end{array}\right\} \tag{21}$$

It is not important exactly which i indices and which j indices are attached to which deltas, because of the symmetry of the diffusion tensor, and because of the symmetrizing effect of the outermost SYM operator in Eq. (20).

After summation over the j indices, terms with s deltas of the first type give rise to a term in the result with $(R/2-q/2)+(q/2-s/2) = (R/2-s/2)$ deltas and with a diffusion tensor having s free indices and $R-s$ contracted indices. We therefore define:

$$U^{(R,s)}_{i_1 i_2\cdots i_R} = \mathop{\mathrm{SYM}}_{i_1 i_2\cdots i_R}\left(\delta_{i_{s+1} i_{s+2}}\cdots\delta_{i_{R-1} i_R}\sum_{j_1 j_2\cdots j_{(R-s)/2}} D_{i_1 i_2\cdots i_s j_1 j_1 j_2 j_2\cdots j_{(R-s)/2} j_{(R-s)/2}}\right) \tag{22}$$

(It follows that $U^{(R,R)}_{i_1 i_2\cdots i_R} = D_{i_1 i_2\cdots i_R}$.)
Substituting Eq. (21) into Eq. (20) gives:

$$D_{i_1 i_2\cdots i_R} = \sum_{q=0,2,\ldots,R}\frac{\alpha(R,q)}{(R+q+1)!}\sum_{s=0,2,\ldots,q}\frac{(R+q)!!q!R!}{(R-s)!!(q-s)!!s!}U^{(R,s)}_{i_1 i_2\cdots i_R} \tag{23}$$

By reversing the order of summation over q and s we obtain:

$$D_{i_1 i_2\cdots i_R} = \sum_{s=0,2,\ldots,R}U^{(R,s)}_{i_1 i_2\cdots i_R} \times\sum_{q=s,s+2,\ldots,R}\frac{\alpha(R,q)q!R!}{(R+q+1)!!(R-s)!!(q-s)!!s!} \tag{24}$$

If we now demand that Eq. (24) is the identity, the factor after $U^{(R,R)}$ has to equal 1 and the factors behind the other $U^{(R,s)}$ have to be 0:

$$\sum_{q=s,s+2,\ldots,R}\frac{\alpha(R,q)q!R!}{(R+q+1)!!(R-s)!!(q-s)!!s!}\begin{cases} = 1 & [s = R] \\ = 0 & [s < R]\end{cases} \tag{25}$$

This is a triangular set of linear equations, which is straightforwardly solved: $\alpha(R,R)$ follows from Eq. (25) with $s = R$; using the solution of $\alpha(R,R)$ and putting $s = R-2$ one can solve $\alpha(R,R-2)$; using $\alpha(R,R)$ and $\alpha(R,R-2)$ and putting $s = R-4$ one can solve $\alpha(R,R-4)$ and so forth. We leave it to the reader to solve the first few coefficients, and see that they all are in agreement with Eq. (13). To check that this is indeed the general expression for $\alpha(R,q)$ we substitute Eq. (13) into Eq. (25). The left hand side of Eq. (25) becomes:

$$\sum_{q=s,s+2,\ldots,R} \frac{(R+q+1)!!}{(R-q)!!q!}(-1)^{\frac{R-q}{2}} \frac{q!R!}{(R+q+1)!!(R-s)!!(q-s)!!s!} \tag{26}$$

Simplifying this and then substituting $h = (R - q)/2$ and $t = (R - s)/2$ yields:

$$\frac{R!}{2^{2t}(R-2t)!t!^2}\sum_{h=0}^{t}(-1)^h\frac{t!}{h!(t-h)!} \tag{27}$$

For $s = R$, $t = 0$ Eq. (27) equals 1. For $s < R$, $t > 0$ the summation in Eq. (27) yields 0; this is a well known series from binomial calculus ([24], it is also a special case of Eq. (A1)). This proves Eq. (13) and we have derived the DTS.

2.4. Odd-order tensors

In the approach of Liu et al. [14] the phases of the diffusion measurement signals, provided they can be measured, obey $\Phi(\boldsymbol{\omega}) = -\Phi(-\boldsymbol{\omega})$ and they are modeled by a sum of odd-order tensors. While this is essentially more complex than the approach in this paper, where the apparent diffusion coefficients are modeled by a single tensor, it might be useful to know that our approach is applicable for odd-order tensors as well.

Following the derivation given above, for odd-order tensors Eqs. (9) and (10) remain unchanged. For Eqs. (12), (14), and (15) q now is odd: $q = 1, 3, \ldots, R$. In Eq. (15) H tensors occur with order $P = R + 1, R + 3, \ldots, 2R$, so P is even, just as in the even-order case. In Eq. (20) $q = 1, 3, \ldots, R$. In Eq. (21) we see that the number of deltas of the first type (i.e. with one i and with one j index) always is odd, so $s = 1, 3, \ldots, q$. The resulting expression is unchanged. Eq. (22) remains the same (now applied with odd s and R). In Eq. (23) the summation indices become: $q = 1, 3, \ldots, R$; $s = 1, 3, \ldots, q$. Reversing the summation order, Eq. (24), gives $s = 1, 3, \ldots, R$; $q = s, s + 2, \ldots, R$. Eqs. (25)–(27) do not change.

So for odd-order tensors the same coefficients $\alpha(R, q)$ and the same solution are obtained as for the even-order tensors, except for the summation over q, which has odd values instead of even.

3. Finite acquisition schemes

3.1. The H tensor check

As mentioned above a (finite) acquisition scheme is a set of directions $\{\mathbf{g}[1], \mathbf{g}[2], \ldots, \mathbf{g}[N]\}$ in which the apparent diffusion coefficient is measured. The $\mathbf{g}[n]$ have to be sufficiently independent, and N has to be equal to or larger than M, being the number of independent elements of the diffusion tensor of order R. We investigate whether there are finite acquisition schemes for which the DTS, as derived above, is valid.

Since both $A(\boldsymbol{\omega})$ (Eq. (9)) and $S(\boldsymbol{\omega})$ (Eqs. (11) and (12)) depend on $\boldsymbol{\omega}$ through $\mathbf{g}(\boldsymbol{\omega})$, we define $A[n]$ and $S[n]$ by replacing $\mathbf{g}(\boldsymbol{\omega})$ by $\mathbf{g}[n]$, giving rise to the following direct tensor solution for a finite acquisition scheme (cf. Eq. (10)):

$$D_{i_1 i_2 \cdots i_R} = \frac{1}{N}\sum_{n=1}^{N} S_{i_1 i_2 \cdots i_R}[n]A[n], \tag{28}$$

where now the solution tensor $S[n]$ is known.

Following the derivation of the DTS of the previous sections, we see that a necessary and sufficient condition for Eq. (28) to be valid, is that Eq. (29), being the discrete version of the H tensor equation (Eq. (19)), holds for all orders $P = R, R + 2, \ldots, 2R$:

$$\frac{1}{N}\sum_{n=1}^{N} g_{i_1}[n]g_{i_2}[n]\cdots g_{i_P}[n] = \frac{1}{P+1}\mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4}\cdots\delta_{i_{P-1} i_P}) \tag{29}$$

Unlike the case with the infinite acquisition scheme, Eq. (29) is not generally valid. Instead it has to be checked for every acquisition scheme. In practice, when checking a particular scheme, it is convenient to use the H function, Eq. (18). Because of the symmetry, one needs to perform only $(P + 1)(P + 2)/2$ tests to check Eq. (29) for order P. In Fig. 3 these tests are explicitly shown for orders $P = 2$ and 4.

Order $P = 2$:

$$\frac{1}{N}\sum_{n=1}^{N} g_i[n]\, g_j[n] = \frac{1}{3}\delta_{ij}$$

$$\begin{cases} \frac{1}{N}\sum g_x^2 = \frac{1}{N}\sum g_y^2 = \frac{1}{N}\sum g_z^2 = \frac{1}{3} \\ \frac{1}{N}\sum g_x g_y = \frac{1}{N}\sum g_y g_z = \frac{1}{N}\sum g_x g_z = 0 \end{cases}$$

Order $P = 4$:

$$\frac{1}{N}\sum_{n=1}^{N} g_i[n]\, g_j[n]\, g_k[n]\, g_l[n] = \frac{1}{15}\delta_{ij}\delta_{kl} + \frac{1}{15}\delta_{ik}\delta_{jl} + \frac{1}{15}\delta_{il}\delta_{jk}$$

$$\begin{cases} \frac{1}{N}\sum g_x^4 = \frac{1}{N}\sum g_y^4 = \frac{1}{N}\sum g_z^4 = \frac{1}{5} \\ \frac{1}{N}\sum g_x^3 g_y = \frac{1}{N}\sum g_y^3 g_z = \frac{1}{N}\sum g_x^3 g_z \\ \quad = \frac{1}{N}\sum g_x g_y^3 = \frac{1}{N}\sum g_y g_z^3 = \frac{1}{N}\sum g_x g_z^3 = 0 \\ \frac{1}{N}\sum g_x^2 g_y^2 = \frac{1}{N}\sum g_y^2 g_z^2 = \frac{1}{N}\sum g_x^2 g_z^2 = \frac{1}{15} \\ \frac{1}{N}\sum g_x^2 g_y g_z = \frac{1}{N}\sum g_x g_y^2 g_z = \frac{1}{N}\sum g_x g_y g_z^2 = 0 \end{cases}$$

Fig. 3. The H tensor check for orders $P = 2$ and 4 and the corresponding $(P + 1)(P + 2)/2$ individual tests to be performed. In the individual equations, the index n has been dropped for clarity.

3.2. Condition numbers

The noise behavior of an acquisition scheme may be described by the condition number, κ [8,16–18]. The smaller κ the better the noise properties. As described in the Introduction, in the traditional solution the independent elements of the diffusion tensor of order R are written as a vector: D_m, $m = 1 \cdots M$, $M = (R + 1)(R + 2)/2$, and Eq. (9) is written as a matrix–vector relationship: $A[n] = \sum_m G_{nm} D_m$. A method to calculate κ [17] defines the matrix $\mathbf{K}$ as the product of G_{nm} with its transpose: $K_{mp} = \sum_n G_{nm} G_{np}$. Then κ equals the square root of the ratio of the largest and smallest eigenvalues of $\mathbf{K}$, i.e. $\kappa = \sqrt{(\varepsilon_{max}/\varepsilon_{min})}$. Although this definition is not in tensor form, it is possible to follow the approach and to calculate κ for the direct tensor solution.

To transform the diffusion tensor $D_{i_1 i_2 \cdots i_R}$ into a vector D_m, we use a list of independent index combinations for a symmetric tensor. For $R = 2$ we have $\{xx, yy, zz, xy, xz, yz\}$, and for $R = 4$ $\{xxxx, yyyy, zzzz, xxyy, xxzz, yyzz, xyyy, xxxy, xyzz, xzzz, xxxz, xyyz, yzzz, yyyz, xxyz\}$, etc. (the order of combinations in the list does not influence the result, as long as it is consequently adhered to). We now put vector component D_m equal to the diffusion tensor element with index combination nr. m from the list:

$$D_m = D_{i_1[m]i_2[m]\cdots i_R[m]}. \tag{30}$$

Then the matrix G_{nm} is given by:

$$G_{nm} = \mu(m) g_{i_1[m]}[n] g_{i_2[m]}[n] \cdots g_{i_R[m]}[n], \tag{31}$$

where $\mu(m)$ is the multiplicity factor, i.e. the number of times the tensor element with indices $(i_1[m], i_2[m], \ldots, i_R[m])$ occurs in a symmetric tensor of order R [7],

$$\mu(m) = \frac{R!}{n_x(m)!n_y(m)!n_z(m)!}, \tag{32}$$

where $n_x(m)$, $n_y(m)$ and $n_z(m)$ are the number of occurrences of x, y and z in $\{i_1[m], i_2[m], \ldots, i_R[m]\}$.

Assuming that the DTS holds, i.e. Eq. (29) is valid, and using the functional expression for the H tensor, Eq. (18), as well as expression (32), the elements of matrix $\mathbf{K}$ are written in closed form:

$$\begin{aligned} K_{mp} &= \sum_{n=1}^{N} G_{nm} \cdot G_{np} \\ &= \sum_{n=1}^{N} \mu(m) g_{i_1[m]}[n] g_{i_2[m]}[n] \cdots g_{i_R[m]}[n] \cdot \mu(p) g_{i_1[p]}[n] g_{i_2[p]}[n] \cdots g_{i_R[p]}[n] \\ &\begin{cases} = \dfrac{R!^2 (n_x(m)+n_x(p)-1)!!(n_y(m)+n_y(p)-1)!!(n_z(m)+n_z(p)-1)!!}{n_x(m)!n_y(m)!n_z(m)!n_x(p)!n_y(p)!n_z(p)!(2R+1)!!} \\ \quad [n_x(m)+n_x(p), n_y(m)+n_y(p), n_z(m)+n_z(p) \text{ even}] \\ = 0 \qquad\qquad [\text{otherwise}] \end{cases} \end{aligned} \tag{33}$$

In Eq. (33) the dependency on the measurement directions is "summated away", so it follows that, for the DTS, $\mathbf{K}$ and κ *are invariant for rotations of the co-ordinate system*. For order 2 we have:

$$\mathbf{K}^{(R=2)} = \frac{1}{15}\begin{pmatrix} 3 & 1 & 1 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 & 0 & 0 \\ 1 & 1 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix} \qquad \kappa^{(R=2)} = \frac{1}{2}\sqrt{10} \approx 1.58114 \tag{34}$$

Both the matrix and the value of $\kappa^{(R=2)}$ are well known [17]. Using the general expression of Eq. (33), however, we may evaluate κ for any order R. For $R = 4$ we obtain:

$$\mathbf{K}^{(R=4)} = \frac{1}{315}\begin{pmatrix} 35 & 3 & 3 & 30 & 30 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 35 & 3 & 30 & 6 & 30 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 3 & 35 & 6 & 30 & 30 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 30 & 30 & 6 & 108 & 36 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 30 & 6 & 30 & 36 & 108 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 6 & 30 & 30 & 36 & 36 & 108 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 80 & 48 & 48 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 48 & 80 & 48 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 48 & 48 & 144 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 80 & 48 & 48 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48 & 80 & 48 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48 & 48 & 144 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 80 & 48 & 48 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48 & 80 & 48 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48 & 48 & 144 \end{pmatrix}$$

$$\kappa^{(R=4)} = \sqrt{\frac{221 + \sqrt{36745}}{221 - \sqrt{36745}}} \approx 3.75235 \tag{35}$$

This is in agreement with the experimental value published recently in a comparison of the noise behavior of acquisition schemes to measure a fourth-order tensor [8].

For $R = 6$ we numerically found the value: $\kappa = 9.835047$.

In conclusion: when the DTS is valid, the condition number of the measurement is invariant under rotations of the co-ordinate system, and its value depends only on the order of the tensor being measured, not on the acquisition scheme used.

3.3. The order of an acquisition scheme

If for an acquisition scheme Eq. (29) is valid for an order P, then it is also valid for orders $P-2, P-4, \ldots$ This can be shown by contracting both sides of Eq. (29) once (i.e. put two indices equal, and summate over them) and working this out algebraically. A direct consequence is that if Eq. (29) is *not* valid for a certain order Q, it will *not* be valid for orders $Q+2, Q+4 \ldots$ either. So when there is an order P for which Eq. (29) is valid, while for order $P+2$ it is not, then P is the maximum order for which Eq. (29) holds, and it follows that the DTS is valid for this acquisition scheme for all orders up to and including $P/2$. We will call this order *the order of the acquisition scheme*, $R_S = P/2$. A finite acquisition scheme must have a finite order R_S, because an upper bound for R_S is given by the condition $(R_S+1)(R_S+2)/2 \leqslant N$.

A well known source for acquisition schemes with directions that are regularly distributed over the sphere, is formed by the vertices of the Platonic and Archimedean solids (Fig. 4, [27,28]). (Although they all possess regularity and symmetry, not all of them are quite homogeneous, as can be seen from the rather large differences in face surfaces of some of the solids in Fig. 4.) With the exceptions of the tetrahedron and the truncated tetrahedron, the number of independent directions in these schemes equals half the number of vertices. We have calculated R_S using exact expressions for the vertices, as can be found in [28], except for the snub cube and the snub dodecahedron, in which case we used a floating point approximation. As depicted in Fig. 4, we find that all Platonic and Archimedean schemes with icosahedral symmetry have $R_S = 2$, the other schemes have $R_S = 1$.

To investigate the rotational invariance of the order of a scheme, we show that if Eq. (29) holds for a order P for a specific scheme, it holds as well when we rotate the scheme (or equivalently when we rotate the co-ordinate system). Let the rotation be given by the matrix operator R_{ij}, and the rotated scheme by $\{\sum_j R_{ij} g_j[n], n = 1 \cdots N\}$, then we have to prove that:

$$\frac{1}{N}\sum_{n=1}^{N} \sum_{j_1 j_2 \cdots j_N} R_{i_1 j_1} g_{j_1}[n] R_{i_2 j_2} g_{j_2}[n] \cdots R_{i_P j_P} g_{j_P}[n] = \frac{1}{P+1} \mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4} \cdots \delta_{i_{P-1} i_P}) \tag{36}$$

Rotating Eq. (36) backwards, i.e. subjecting both sides to

$$\sum_{i_1 i_2 \cdots i_P} R^{-1}_{k_1 i_1} R^{-1}_{k_2 i_2} \cdots R^{-1}_{k_P i_P}(\cdot), \tag{37}$$

and, using the orthogonality of the rotation, $R^{-1}_{ij} = R_{ji}$, we obtain

$$\begin{aligned} &\frac{1}{N}\sum_{n=1}^{N} g_{k_1}[n] g_{k_2}[n] \cdots g_{k_P}[n] \\ &= \sum_{i_1 i_2 \cdots i_P} R^{-1}_{k_1 i_1} R^{-1}_{k_2 i_2} \cdots R^{-1}_{k_P i_P} \frac{1}{P+1} \mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4} \cdots \delta_{i_{P-1} i_P}) \\ &= \frac{1}{P+1} \mathrm{SYM}\left(\sum_{i_1 i_2 \cdots i_P} R^{-1}_{k_1 i_1} \delta_{i_1 i_2} R_{i_2 k_2} R^{-1}_{k_3 i_3} \delta_{i_3 i_4} R_{i_4 k_4} \cdots R^{-1}_{k_{P-1} i_{P-1}} \delta_{i_{P-1} i_P} R_{i_P k_P} \right) \\ &= \frac{1}{P+1} \mathrm{SYM}(\delta_{k_1 k_2}\delta_{k_3 k_4} \cdots \delta_{k_{P-1} k_P}), \end{aligned} \tag{38}$$

which is Eq. (40) again. So if Eq. (40) holds for an acquisition scheme for order P, it also holds for the rotated scheme for order P, and therefore the DTS for order $R = P/2$ holds as well. We conclude that *the order of an acquisition scheme is a rotationally invariant parameter*.

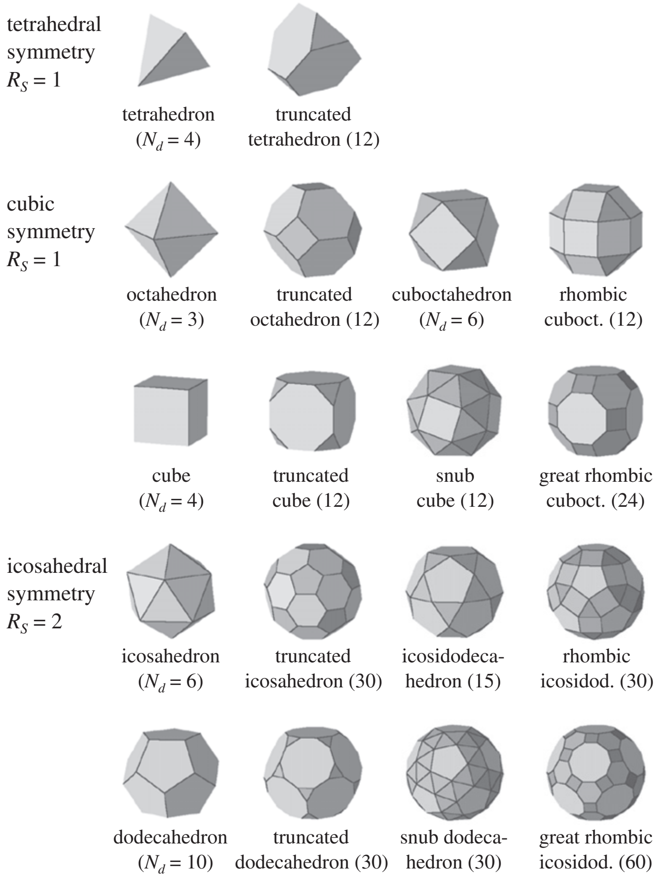

Fig. 4. Acquisition schemes determined by the vertices of the Platonic solids (first column) and the Archimedean solids (other columns). With every scheme the number of directions of the scheme, N_d, is given in parentheses. R_S is the order of the scheme, i.e. the maximum order for which the direct tensor solution is valid.

3.4. Weighted acquisition schemes

Searching for schemes with a higher order, we investigated the tessellations of the icosahedron, which are being regularly used in literature [7,9,17,18,29]. Rather disappointingly, though, all tessellations we checked have order 2. As described in the caption of Fig. 5, this can be understood by the fact that tessellations of the icosahedron are essentially inhomogeneous; they do not converge to the infinite acquisition scheme, which is homogeneous per definition.

Our way to obtain acquisition schemes with a higher order follows from the observation that the direct tensor solution in a finite acquisition scheme may be seen as a discrete approximation of the continuous (integral) solution of the infinite scheme. In such an approximation one should take into account the variable of integration $d\boldsymbol{\omega}$: each direction in the finite scheme represents a solid angle. Therefore we introduce weighting factors, $w[n]$, connected to the directions, with $w[n]/N$ in the finite scheme corresponding to $d\boldsymbol{\omega}/4\pi$ in the infinite scheme. Eq. (28) then becomes:

$$D_{i_1 i_2 \cdots i_R} = \frac{1}{N}\sum_{n=1}^{N} S_{i_1 i_2 \cdots i_R}[n]A[n]w[n], \tag{39}$$

and Eq. (29) is modified into:

$$\frac{1}{N}\sum_{n=1}^{N} g_{i_1}[n]g_{i_2}[n]\cdots g_{i_P}[n]w[n] = \frac{1}{P+1}\mathrm{SYM}(\delta_{i_1 i_2}\delta_{i_3 i_4}\cdots\delta_{i_{P-1} i_P}) \tag{40}$$

It can easily be checked that like Eq. (29) also Eq. (40) has the property that if it is holds for order P, it also holds for orders $P-2, P-4, \ldots$, so everything we derived about the order of an acquisition scheme, remains valid for a weighted acquisition scheme.

To calculate the condition number of a weighted acquisition scheme, we introduce the $N \times N$ diagonal matrix $\mathbf{U}$, with $U_{nn} = \sqrt{w[n]}$. For the $\mathbf{K}$-matrix we now have $\mathbf{K} = (\mathbf{GU})^{\mathrm{T}}(\mathbf{GU})$ and Eq. (33) holds in the same way, with the same resulting condition numbers as in the non weighted case.

Since in the Platonic and Archimedean schemes all directions are equivalent, i.e. the vertices are indistinguishable, there is no useful way to introduce weighting factors, since there is no sensible way to label one direction with a different weighting factor than another. The vertices of the tessellations of the icosahedron, however, are distinguishable. It is possible to divide these schemes into subsets of equivalent points, so different weighting factors can be attributed to each subset.

Let us suppose in a specific scheme there are m different subsets and therefore m different weighting factors. Applying Eq. (40) for an order P gives a set of linear equations with m unknowns. Choosing the order too low gives an underdetermined set of equations, choosing the order too high gives an inconsistent set of equations. The highest order which produces a solvable set of equations determines the order of the acquisition scheme, $R_S = P_{\max}/2$, as well as the values of the weighting factors.

Fig. 6 shows the results for a number of tessellations of the icosahedron as well as for the combination of icosahedron and dodecahedron. This is a useful scheme with less directions than the 1x tessellated icosahedron, while still possessing order 4. We see that with the use of weighting factors schemes with higher orders can indeed be obtained.

4. Additional results

4.1. Relations between tensors of different orders

If we measure a voxel whose diffusion properties are governed by a diffusion tensor of order R,

$$A^{(R)}(\boldsymbol{\omega}) = \sum_{i_1 i_2 \cdots i_R} g_{i_1}(\boldsymbol{\omega})g_{i_2}(\boldsymbol{\omega})\cdots g_{i_R}(\boldsymbol{\omega})D_{i_1 i_2 \cdots i_R}, \tag{41}$$

and we use these values to calculate a diffusion tensor of order T,

$$D^{(R\to T)}_{i_1 i_2 \cdots i_T} = \frac{1}{4\pi}\int_{\Omega} S_{i_1 i_2 \cdots i_T}(\boldsymbol{\omega})A^{(R)}(\boldsymbol{\omega})d\boldsymbol{\omega}, \tag{42}$$

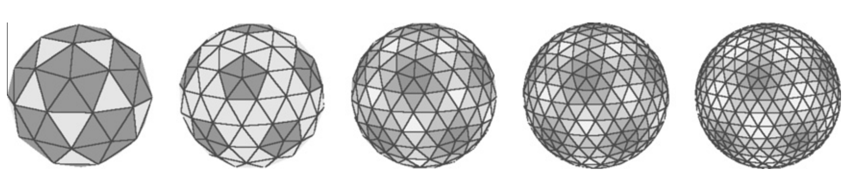

Fig. 5. Tessellations of the icosahedron: from left to right 1 to 5 times tessellated. Smaller faces are rendered darker than bigger ones, so in the darker areas the density of vertices is larger than in the lighter areas. One sees that for increasing degree of tessellation the vertex density close to the original vertices of the icosahedron remains higher, illustrating the tessellations do not converge to a homogeneous scheme, and therefore do not converge to the infinite acquisition scheme.

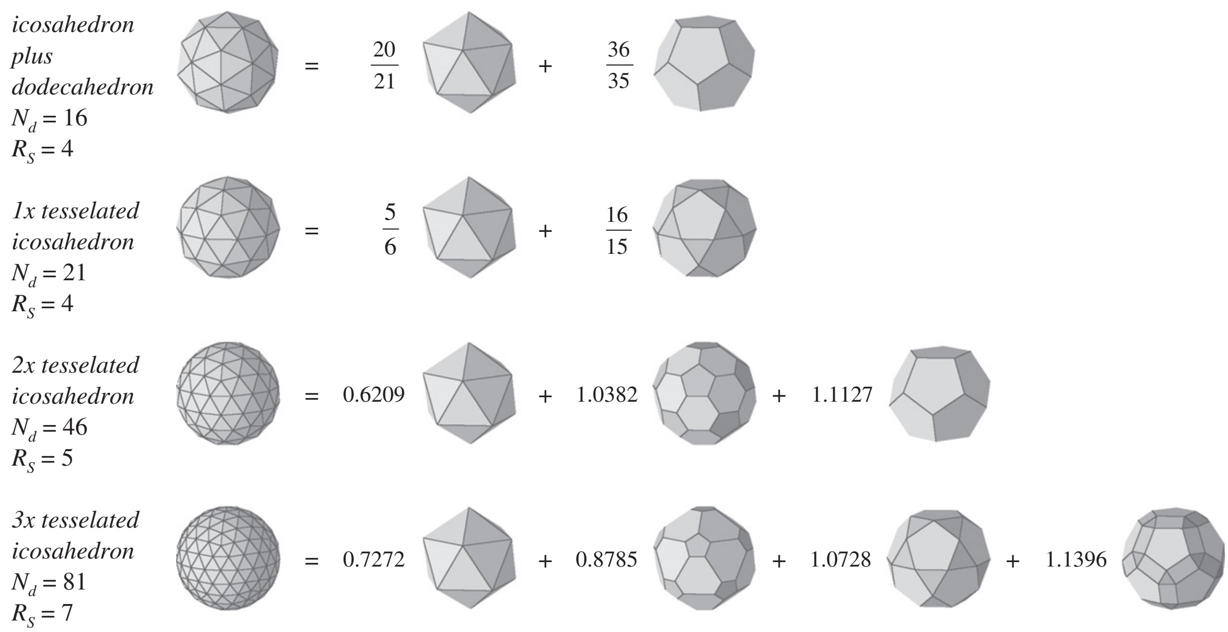

Fig. 6. Acquisition schemes with subsets and weighting factors per subset. With every scheme the number of independent directions, N_d, and the order of the scheme, R_S, are listed. Weighting factors are mentioned after the = sign together with a representation of their subsets.

then substitution of Eq. (41) into Eq. (42) gives a natural relationship between two diffusion tensors of different order.

Working this out, analogously to the derivation of the DTS, but using the DTS itself (Eqs. (11)–(13)), we obtain the following expression:

$$D^{(R\to T)}_{i_1 i_2 \cdots i_T} = \sum_{s=0,2,\ldots,\min(R,T)} \beta(T,R,s) U^{(T,R,s)}_{i_1 i_2 \cdots i_T}(\boldsymbol{\omega}), \tag{43}$$

with the coefficients $\beta(T,R,s)$ obeying:

$$\beta(T,R,s) = \frac{R!}{(R-s)!!s!} \times \sum_{q=s,s+2,\ldots,T} (-1)^{\frac{T-q}{2}} \frac{(T+q+1)!!}{(T-q)!!(R+q+1)!!(q-s)!!}, \tag{44}$$

and where the tensor $U^{(T,R,s)}$ is a generalization of $U^{(R,s)}$ (Eq. (22)): $U^{(T,R,s)}$ is a tensor of order T, consisting of a diffusion tensor of order R which is contracted $(R-s)/2$ times (thus having order s), supplemented with $(T-s)/2$ deltas to obtain a tensor of order T, which is finally symmetrized:

$$U^{(T,R,s)}_{i_1 i_2 \cdots i_T} = \underset{i_1 i_2 \cdots i_T}{\mathrm{SYM}} \left(\delta_{i_{s+1} i_{s+2}} \cdots \delta_{i_{T-1} i_T} \sum_{j_1 j_2 \cdots j_{(R-s)/2}} D_{i_1 i_2 \cdots i_s j_1 j_1 j_2 j_2 \cdots j_{(R-s)/2} j_{(R-s)/2}} \right). \tag{45}$$

We first evaluate Eq. (44) for $T > R$. Dividing the factor $(T+q+1)!!$ by $(R+q+1)!!$ leaves a polynomial in q in the numerator behind the summation sign. We substitute $k = (q-s)/2$ for q, and rewrite the remaining double factorials behind the summation sign as ordinary factorials (with help of Eq. (8)):

$$\beta(T,R,s) = \frac{R!}{(R-s)!!s!} (-1)^{\frac{T-s}{2}} 2^{\frac{s-R}{2}} \times \sum_{k=0}^{\frac{T-s}{2}} (-1)^k \frac{\left(\frac{T+s+1}{2}+k\right)\left(\frac{T+s-1}{2}+k\right)\cdots\left(\frac{R+s+3}{2}+k\right)}{\left(\frac{T-s}{2}-k\right)!k!}. \tag{46}$$

The series is equivalent to Eq. (A2) from Appendix A, with $N = (T-s)/2$. The degree of the polynomial in k in the numerator behind the summation sign equals $(T-R)/2$, which is always smaller than N, except for $s = R$, when it equals N, and only in that case the result is unequal to zero. A little algebra yields:

$$\beta(T,R,s) = \begin{cases} 1 & [s = R, T > R] \\ 0 & [s < R, T > R] \end{cases} \tag{47}$$

and Eq. (43) takes a relatively simple form:

$$D^{(R\to T)}_{i_1 i_2 \cdots i_T} = \mathrm{SYM}(D_{i_1 i_2 \cdots i_R} \delta_{i_{R+1} i_{R+2}} \cdots \delta_{i_{T-1} i_T}) \quad [T > R] \tag{48}$$

In words: to express a diffusion tensor of order R in terms of a tensor with a higher order T, supplement it with deltas to get a tensor of order T, and symmetrize.

Following the same steps for $T < R$, an extra polynomial arises in the *denominator* behind the summation sign, which makes the evaluation of Eq. (44) considerably more complex. We confine ourselves to the case $T = R - 2$. In that case, dividing $(T+q+1)!!$ by

$$D^{(0\to2)}_{ij} = D\,\delta_{ij} \qquad D^{(2\to0)} = \tfrac{1}{3}\sum_a D_{aa}$$

$$D^{(2\to4)}_{ijkl} = \mathrm{SYM}(D_{ij}\,\delta_{kl}) \qquad D^{(4\to2)}_{ij} = -\tfrac{3}{35}\delta_{ij}\sum_{ab} D_{aabb} + \tfrac{6}{7}\sum_a D_{ijaa}$$

$$D^{(4\to6)}_{ijklmn} = \mathrm{SYM}(D_{ijkl}\,\delta_{mn}) \qquad D^{(6\to4)}_{ijkl} = \tfrac{5}{231}\mathrm{SYM}(\delta_{ij}\delta_{kl})\sum_{abc} D_{aabbcc} - \tfrac{5}{11}\mathrm{SYM}\left(\delta_{ij}\sum_{ab} D_{klaabb}\right) + \tfrac{15}{11}\sum_a D_{ijklaa}$$

$$D^{(6\to8)}_{ijklmnpq} = \mathrm{SYM}(D_{ijklmn}\,\delta_{pq}) \qquad D^{(8\to6)}_{ijklmn} = -\tfrac{7}{1287}\mathrm{SYM}(\delta_{ij}\delta_{kl}\delta_{mn})\sum_{abcd} D_{aabbccdd} + \tfrac{28}{142}\mathrm{SYM}\left(\delta_{ij}\delta_{kl}\sum_{abc} D_{mnaabbcc}\right) - \tfrac{14}{13}\mathrm{SYM}\left(\delta_{ij}\sum_{ab} D_{klmnaabb}\right) + \tfrac{28}{15}\sum_a D_{ijklmnaa}$$

Fig. 7. Examples of relations between tensors of different orders.

$(R+q+1)!!$ leaves a factor $R+q+1$ in the denominator. Substituting again $k=(q-s)/2$ for q and rewriting the double factorials into ordinary factorials:

$$\beta(R-2,R,s) = \frac{R!}{(R-s)!!s!}(-1)^{\frac{R-s-2}{2}}2^{\frac{s-R}{2}}\sum_{k=0}^{\frac{R-s-2}{2}}\frac{(-1)^k}{\left(\frac{R+s}{2}+k+\frac{1}{2}\right)\left(\frac{R-s-2}{2}-k\right)!k!} \tag{49}$$

Applying Eq. (A5) from the appendix, with $j=(R+s)/2$ and $N=(R-s-2)/2$, we find:

$$\beta(R-2,R,s) = \frac{R!(R+s-1)!!}{(R-s)!!s!(2R-1)!!}(-1)^{\frac{R-s-2}{2}}, \tag{50}$$

which substituted into Eq. (43) yields the expression for $D^{(R\to R-2)}$.

Fig. 7 shows some of these relationships explicitly worked out for orders 0, 2, 4 and 6. We observe that two special cases of these relationships were deduced before. Özarslan and Mareci [7] found expressions for $D^{(6\to 4)}$ and $D^{(4\to 2)}$, using spherical harmonics; not in the tensor form we present here, however, but in the form of tabulated relations between tensor elements. Moakher [12] derived the expression for $D^{(4\to 2)}$ in tensor form.

4.2. The Platonic Variance Property

The Platonic Variance Property as introduced in [22] is defined as:

$$\overline{A} = \overline{\lambda}, \quad \mathrm{Var}\,A = \frac{2}{5}\mathrm{Var}\,\lambda, \tag{51}$$

where λ denotes the eigenvalues of the second-order diffusion tensor and A the measured apparent diffusion coefficients. With this property a number of scalar invariants, like the Fractional Anisotropy, can be efficiently expressed as direct functions of the $A[n]$. In [22] some acquisition schemes were presented that possess this property. Using the results of the present paper, however, we can make more general statements.

Let us rewrite Eq. (51) in terms of the second-order diffusion tensor:

$$\overline{A} = \frac{1}{3}\sum_i D_{ii}; \quad \overline{A^2} - \overline{A}^2 = \frac{2}{5}\left\{\frac{1}{3}\sum_{ij} D_{ij}^2 - \left(\frac{1}{3}\sum_i D_{ii}\right)^2\right\}. \tag{52}$$

For the second-order diffusion measurement we have:

$$A[n] = \sum_{ij} g_i[n]g_j[n]D_{ij}. \tag{53}$$

Using Eq. (53) we evaluate Mean A and Mean A^2, taking into account the weighting factors for a weighted acquisition scheme:

$$\begin{aligned}\overline{A} &= \frac{1}{N}\sum_{n=1}^{N} w[n]A[n] = \sum_{ij} D_{ij}\frac{1}{N}\sum_{n=1}^{N} g_i[n]g_j[n]w[n] = \sum_{ij} D_{ij}\frac{1}{3}\delta_{ij}\\ &= \frac{1}{3}\sum_i D_{ii},\end{aligned} \tag{54}$$

$$\begin{aligned}\overline{A^2} &= \frac{1}{N}\sum_{n=1}^{N} w[n]\sum_{ij} g_i[n]g_j[n]D_{ij}\sum_{kl} g_k[n]g_l[n]D_{kl}\\ &= \sum_{ij}\sum_{kl} D_{ij}D_{kl}\frac{1}{N}\sum_{n=1}^{N} g_i[n]g_j[n]g_k[n]g_l[n]w[n]\\ &= \sum_{ij}\sum_{kl} D_{ij}D_{kl}\frac{1}{15}\{\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\}\\ &= \frac{1}{15}\left(\sum_i D_{ii}\right)^2 + \frac{2}{15}\sum_{ij} D_{ij}^2\end{aligned} \tag{55}$$

Eqs. (54) and (55) are equivalent to Eq. (52). The essential point is, that we used the H tensor equation for order 2 (Eq. (54)) and for order 4 (Eq. (55)). The conclusion therefore is that *the Platonic Variance Property holds for all* (*weighted*) *acquisition schemes with order* $R_S \geqslant 2$.

Furthermore, by inspection of Eqs. (54) and (55) we arrive at the conclusion that, if we want to extend the Platonic Variance Method to calculate scalars which are polynomials of degree 3 of the eigenvalues (e.g. Skewness), and we consequently require that Mean A^3 be a rotationally invariant function of the diffusion tensor, we need to use an acquisition scheme with order $R_S \geqslant 3$.

5. Discussion

Our first question was: *Does there exist a general expression for the inverse of* Eq. (3) *that preserves the tensor form*? The question has been answered in the affirmative. The DTS is derived algebraically as an exact linear expression, which, resubstituted in Eq. (3) yields the identity equation. The traditional solution has the same properties and it follows that in acquisition schemes where the direct tensor solution holds, it must be equal to the traditional solution. In this respect the direct tensor solution is not a new tool for the actual calculation of the tensor from measured data (although it can be used for this purpose: see Appendix B). Its true value lies in the tensor form, and in the ensuing properties and insights.

With respect to the form of the solution tensor, we argued that it should be built up out of unit vectors, $g_i(\boldsymbol{\omega})$, and Kronecker deltas, δ_{ij}. We restricted ourselves, however, to using the operations: addition, tensor multiplication and multiplication by real numbers. Although the fact that a solution indeed was found may be seen as a justification for this approach, questions about its generality might arise. In principle three extra possibilities to construct the solution tensor exist: multiplication by scalars that are a function of the direction $\boldsymbol{\omega}$, integration over $\boldsymbol{\omega}$, and contraction of indices. A scalar function of $\boldsymbol{\omega}$ might be obtained by contracting a pair of $g_i(\boldsymbol{\omega})$. Since $\sum_i g_i(\boldsymbol{\omega})g_i(\boldsymbol{\omega})=1$, however, this is not a useful option. Because of the H tensor equation (Eq. (19)), integrating a number of $g_i(\boldsymbol{\omega})$ over $\boldsymbol{\omega}$ yields an expression in δ_{ij}, which is covered already by our approach. Likewise do the remaining possible contractions fail to yield something new: $\sum_i g_i(\boldsymbol{\omega})\delta_{ij} = g_j(\boldsymbol{\omega})$, $\sum_i \delta_{ii} = 3$, $\sum_i \delta_{ij}\delta_{ik} = \delta_{jk}$. Therefore there are no possibilities known to us, which could provide a more general form of the solution tensor than the one derived in this paper.

We turn to our second question: *Can we use this expression to formulate mathematical properties and a simple checking procedure for acquisition schemes with a rotationally invariant condition number?* Indeed, we have found the following properties:

- If for an acquisition scheme the H tensor equation for order P holds, then the DTS is valid for all orders $R \leqslant P/2$. Checking if the H tensor equation holds requires testing $(P+1)(P+2)/2$ algebraic equations.
- There is a maximum order for which the DTS is valid; this is called the order of the acquisition scheme, R_S, which is a rotationally invariant parameter.
- If for a specific acquisition scheme the DTS is valid, then the condition number is rotationally invariant and it depends only on the order of the tensor to be measured, not on the acquisition scheme.
- The introduction of weighted acquisition schemes opens the possibility of constructing schemes with higher orders, by solving a set of linear equations.

This is a great improvement compared to the way acquisition schemes have been analyzed thus far. The procedures presented facilitate the use of acquisition schemes with rotationally invariant condition numbers such that reasons to use improper schemes disappear. We expect this will be a valuable tool in the study of crossing fibers, using fourth-order tensors, as well as in possible future applications of higher order GDTI.

Concerning the variations in noise behavior of a GDTI measurement, two effects must be considered separately. First there are rotations of the co-ordinate system relative to the physical setup, which we have considered above. This purely mathematical operation should have no effect on the outcomes of any physical measurement. Since with respect to the acquisition scheme, the noise behavior is characterized by the condition number, the rotational invariance of the condition number is a prerequisite for a proper acquisition scheme. The second source of variations in the noise originates from rotations of the tensor being measured, relative to the acquisition scheme (or vice versa). With the exception of isotropic diffusion, such rotations always give variations in the noise behavior, since they are caused by the finiteness of the scheme; only an infinite scheme would be invariant in this respect. It is therefore not realistic to require rotational invariance of this second effect.

We described two more applications of the direct tensor solution. First there are the relations between tensors of different order. For some specific cases such relations have been derived before [7]; our expressions, however, have a larger generality and they are, of course, in tensor form. Second there is the Platonic Variance Method, which we previously derived for a few specific acquisition schemes [22]. The direct tensor solution tells us that it is valid for all second-order schemes, and shows at the same time how this method can be extended by using higher-order acquisition schemes. Although these applications surely have their practical use, they demonstrate above all the value of the direct tensor solution as a tool to increase our mathematical insight in GDTI.

Throughout this paper we have seen that the H tensor equation plays a pivotal rule; it is used in the derivation of the direct tensor solution, and in every of the applications we presented. To test if the direct tensor solution is valid for a finite acquisition scheme, testing the H tensor equation is sufficient. To our knowledge this equation has not appeared in literature before, and certainly not in the context of GDTI, which is remarkable, considering its elegance and generality.

A shortcoming of the work presented here is that the higher-order acquisition schemes are limited to tessellations of the icosahedron. There exist methods to generate more homogeneous acquisition schemes, like simulated electrostatic repulsion [21,30]. It is not clear, however, how and if weighting factors can be attributed to such schemes. In [29], concerning the integration of spherical harmonic functions, it was suggested, that "the weights in the summation that approximate the integral are equal to the Voronoi areas for the sampling points on the unit sphere". We did some preliminary checks on the tessellated icosahedra, but the weighting factors obtained from the Voronoi areas seem to not exactly equal the weighting factors derived in this paper. This remains a task for future investigations.

An important issue is raised by the fact that diffusion tensors always are positive semidefinite (PSD). In the presence of noise, neither the traditional method nor the direct tensor solution guarantee that the resulting diffusion tensor is PSD. An alternative method for the measurement of fourth-order diffusion tensors, which preserves PSDness, is based on a reparametrization of the traditional method [9,11,31]. We expect that the combination of this method, with the proper acquisition schemes as presented in this paper, will take advantage of the rotational invariance properties. This issue, however, needs further investigation.

Another approach to preserve PSDness uses Riemannian geometry and log-Euclidean metrics. In [32–34] this is applied in the manipulation of second-order tensors (like adding and interpolating). When used to estimate fourth-order tensors [35], however, the fourth-order tensor is regrouped into a second-order tensor in a six dimensional space, which is the kind of procedure we have tried to avoid. So it is unclear at this moment, whether the Riemannian approach can be reconciled with the DTS.

In conclusion: we have presented the Direct Tensor Solution, which is a new equation in tensor form that is the inversion of the basic equation of (generalized) diffusion tensor MRI. The DTS gives a number of interesting new mathematical insights, the most important of which is about the analysis and design of acquisition schemes with a condition number that is rotationally invariant. This may have immediate practical consequences in the measurement of higher-order diffusion tensors.

Appendix A. Series

The basis for the series in Eqs. (46) and (49) can be found in [36]. Here we give both a form which is similar to that in [36] (Eqs. (A1) and (A3)), and a form that we use in this paper (Eqs. (A2) and (A5)).

Ref. [36] Eq. (6.6.3):

$$\sum_{k=0}^{N}(-1)^k\binom{N}{k}(a_0+a_1k+\cdots+a_mk^m) = \begin{cases} 0 & [m<N] \\ (-1)^N N!a_m & [m=N] \end{cases} \quad [N>0] \tag{A1}$$

Division by $N!$ yields:

$$\sum_{k=0}^{N}\frac{(-1)^k}{(N-k)!k!}(a_0+a_1k+\cdots+a_mk^m) = \begin{cases} 0 & [m<N] \\ (-1)^N a_m & [m=N] \end{cases} \quad [N>0] \tag{A2}$$

Ref. [36] Eq. (6.6.8), where $P_m(k)$ is a polynomial in k of degree m:

Order 2:

$$S_{xx}=\tfrac{15}{2}x^2-\tfrac{3}{2} \qquad S_{yy}=\tfrac{15}{2}y^2-\tfrac{3}{2} \qquad S_{zz}=\tfrac{15}{2}z^2-\tfrac{3}{2}$$

$$S_{xy}=\tfrac{15}{2}xy \qquad S_{xz}=\tfrac{15}{2}xz \qquad S_{yz}=\tfrac{15}{2}yz$$

Order 4:

$$S_{xxxx}=\tfrac{315}{8}x^4-\tfrac{105}{4}x^2+\tfrac{15}{8} \qquad S_{xxxy}=\tfrac{315}{8}x^3y-\tfrac{105}{8}xy$$

$$S_{yyyy}=\tfrac{315}{8}y^4-\tfrac{105}{4}y^2+\tfrac{15}{8} \qquad S_{xyyy}=\tfrac{315}{8}xy^3-\tfrac{105}{8}xy$$

$$S_{zzzz}=\tfrac{315}{8}z^4-\tfrac{105}{4}z^2+\tfrac{15}{8} \qquad S_{xxxz}=\tfrac{315}{8}x^3z-\tfrac{105}{8}xz$$

$$S_{xxyz}=\tfrac{315}{8}x^2yz-\tfrac{35}{8}yz \qquad S_{xzzz}=\tfrac{315}{8}xz^3-\tfrac{105}{8}xz$$

$$S_{xyyz}=\tfrac{315}{8}xy^2z-\tfrac{35}{8}xz \qquad S_{yyyz}=\tfrac{315}{8}y^3z-\tfrac{105}{8}yz$$

$$S_{xyzz}=\tfrac{315}{8}xyz^2-\tfrac{35}{8}xy \qquad S_{yzzz}=\tfrac{315}{8}yz^3-\tfrac{105}{8}yz$$

$$S_{xxyy}=\tfrac{315}{8}x^2y^2-\tfrac{35}{8}x^2-\tfrac{35}{8}y^2+\tfrac{5}{8}$$

$$S_{xxzz}=\tfrac{315}{8}x^2z^2-\tfrac{35}{8}x^2-\tfrac{35}{8}z^2+\tfrac{5}{8}$$

$$S_{yyzz}=\tfrac{315}{8}y^2z^2-\tfrac{35}{8}y^2-\tfrac{35}{8}z^2+\tfrac{5}{8}$$

Fig. 8. Elements of the direct solution tensor for orders 2 and 4, expressed in the Cartesian components of $\mathbf{g}(\boldsymbol{\omega})$: $x=g_x(\boldsymbol{\omega})$, $y=g_y(\boldsymbol{\omega})$ and $z=g_z(\boldsymbol{\omega})$, so $x^2+y^2+z^2=1$.

$$\sum_{k=0}^{N}(-1)^k\binom{N}{k}\frac{1}{a+k}P_m(x-k)=\frac{N!\Gamma(a)}{\Gamma(N+a+1)}P_m(x+a)\quad [m\leqslant N] \tag{A3}$$

In Eq. (49) the polynomial P_m equals 1 and a is a half odd integer: $a = j + 1/2$. For this case, Eq. (A3) can be rewritten, using

$$\Gamma\left(n+\frac{1}{2}\right)=\frac{\sqrt{\pi}}{2^n}(2n-1)!! \tag{A4}$$

([24]: 8.339.2), as:

$$\sum_{k=0}^{N}\frac{(-1)^k}{(N-k)!k!}\cdot\frac{1}{j+k+\frac{1}{2}}=\frac{(2j-1)!!}{(2N+2j+1)!!}2^{N+1} \tag{A5}$$

Appendix B. Solution tensors in Cartesian co-ordinates

When one uses an acquisition scheme, with the directions given in Cartesian co-ordinates, and one wants to use the DTS to calculate the diffusion tensor (Eqs. (28) and (39)), Fig. 8 may be useful: it gives the elements of the solution tensor for order 2 and 4, expressed in the Cartesian components of $\mathbf{g}(\boldsymbol{\omega})$.

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