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# Decomposition of High Angular Resolution Diffusion Images into a Sum of Self-Similar Polynomials on the Sphere

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## Abstract

We propose a tensorial expansion of high resolution diffusion imaging (HARDI) data on the unit sphere into a sum of self-similar polynomials, i.e. polynomials that retain their form up to a scaling under the act of lowering resolution via the diffusion semigroup generated by the Laplace-Beltrami operator on the sphere. In this way we arrive at a hierarchy of HARDI degrees of freedom into contravariant tensors of successive ranks, each characterized by a corresponding level of detail. We provide a closed-form expression for the scaling behaviour of each homogeneous term in the expansion, and show that classical diffusion tensor imaging (DTI) arises as an asymptotic state of almost vanishing resolution.

**CR Categories:** I.4.10 [Computing Methodologies]: Image Representation—Multidimensional

**Keywords:** high angular resolution diffusion imaging (HARDI), diffusion tensor imaging (DTI), self-similar polynomials on the sphere

## 1 Introduction

High angular resolution diffusion imaging (HARDI) has become a popular magnetic resonance imaging (MRI) technique for imaging apparent water diffusion processes in fibrous tissues in vivo, such as brain white matter and muscle. Diffusion MRI is based on the assumption that Brownian motion of  $H_2O$  molecules is facilitated along the direction of fibers (axons or muscles). In classic diffusion tensor imaging (DTI), introduced by Basser et al. [Basser et al. 1994a; Basser et al. 1994b], cf. also Le Bihan et al. [Le Bihan et al. 2001], the diffusivity profile is modeled by a rank-2 contravariant diffusion tensor. Although the DTI representation is inherently limited by this restrictive assumption on the diffusivity profile, it does have the advantage that it enables one to view a spatial section of local diffusivity profiles as a (dual) Riemannian metric field. In turn, this view has led to the geometric rationale, in which fibers are modeled as (subsets of) geodesics induced by parallel transport under the corresponding metric connection [Astola et al. 2007; Fillard et al. 2007; Lenglet et al. 2004; Pennec et al. 2006; Prados et al. 2006]. Congruences of geodesics can be studied likewise in the geometric framework of Hamilton-Jacobi theory [Rund 1973], which has led to efficient algorithms for connectivity analysis (eikonal equation, fast marching schemes, and the like).

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For simplicity we use the term HARDI to collectively denote schemes that employ functions on the sphere, including Tuch’s orientation distribution function (ODF) [Tuch 2004], the higher order diffusion tensor model and the diffusion orientation transform (DOT) by Özarslan et al. [Özarslan and Mareci 2003; Özarslan et al. 2006], Q-Ball imaging [Descoteaux et al. 2007], and the diffusion tensor distribution model by Jian et al. [Jian et al. 2007].

Because the general HARDI model accounts for arbitrarily complex diffusivity profiles, it raises a concomitant demand for regularization [Descoteaux et al. 2006; Descoteaux et al. 2007; Hess et al. 2006; Pennec et al. 2006; Tikhonov and Arseninn 1977], since there is no a priori smoothness of acquisition data. Indeed, in the context of regularization schemes, DTI can be seen as an asymptotic regularization of the actual diffusivity profile.

A natural way to combine the conceptual advantage of DTI (notably its connection to a Riemannian framework) with the superior data modeling capability of HARDI, is to consider a polynomial expansion of the diffusivity function on the sphere that can be likewise represented in terms of a contravariant rank-2 tensor field, which can then be used so as to obtain a generalized, orientation dependent Finsler metric [Melonakos et al. 2008]. A polynomial expansion of HARDI data on the sphere has been proposed previously by Özarslan and Mareci [Özarslan and Mareci 2003]. However, these authors consider a *homogeneous* expansion, containing terms of some *fixed* order only. They point out that any (again homogeneous) model of lower order can be obtained in analytically closed form from the result, i.e. without the need for a data refit. This is true, and indeed a sensible approach, since (even/odd) monomials of fixed order,  $N$  say, confined to the unit sphere, can be linearly combined so as to produce any lower order (even/odd) monomial by virtue of the radial constraint  $r = 1$  of the unit sphere embedded in Euclidean  $n$ -space (in our case,  $n = 3$ ).

However, in this paper we propose an *inhomogeneous* expansion, including all (even) orders up to some fixed  $N$ , and exploit the redundancy of such a representation. (Odd terms are of no interest, as the HARDI profile is assumed to be symmetric.) The idea is to construct a polynomial on the sphere in such a way that the higher order terms capture *residual* information of the HARDI profile only, i.e. the additional structure that cannot be revealed by a lower order polynomial. As such the polynomial expansion can in theory be continued to a series expansion of infinite order. We construct this polynomial representation order by order, in such a way that adding a higher order term does not affect already established lower order terms. As a consequence the information in the HARDI data is distributed hierarchically over diffusion tensor coefficients of all ranks.

The polynomial representation admits regularization. This provides control over complexity and angular resolution. Above all, it reveals the data hierarchy alluded to above, in the sense that the collective terms of fixed order are self-similar under canonical resolution degradation induced by the Laplace-Beltrami operator on the sphere (cf. Koenderink for a physical motivation of this paradigm in the Euclidean setting [Koenderink 1984]), with a characteristic decay that depends on order. In this sense they constitute the tensorial counterparts of the canonical eigensystem of spherical harmonics with corresponding discrete spectrum.

Finally, we point out the explicit relationship between HARDI and DTI via asymptotic regularization. This is of interest, as it permits one to extend and apply established geometric techniques for connectivity analysis and tractography that have been successfully used in the context of classical rank-2 DTI.

## 2 Theory

We consider the unit sphere embedded in Euclidean 3-space, given in terms of the vector components  $g^i$ ,  $i = 1, \dots, n$  (with  $n = 3$  in our application of interest):

$$\eta_{ij} g^i g^j = 1. \quad (1)$$

Einstein summation convention applies to pairs of identical upper and lower indices. The components of the Euclidean metric and corresponding dual metric of the embedding space are given by  $\eta_{ij}$ , respectively  $\eta^{ij}$ , with the help of which indices can be lowered or raised. We have, for instance<sup>1</sup>,  $g_i = \eta_{ij} g^j$ , the dual covector components corresponding to  $g^i$ . The corresponding analogue of Eq. (1) is therefore

$$\eta^{ij} g_i g_j = 1. \quad (2)$$

In Cartesian coordinates we have  $\eta_{ij} = \eta^{ij} = 1$  iff  $i = j$  for  $i, j = 1, \dots, n$ , otherwise 0, so that Eq. (2) reduces to  $g_1^2 + g_2^2 + g_3^2 = 1$ , and similarly for the vectorial representation, Eq. (1).

The Riemannian metric of the embedded unit sphere is given in terms of the components

$$g_{\mu\nu} = \frac{\partial g^i}{\partial \xi^\mu} \eta_{ij} \frac{\partial g^j}{\partial \xi^\nu}, \quad (3)$$

in which  $\xi^\mu$  ( $\mu = 1, \dots, n-1$ ) parameterize the sphere. Recall that the canonical parametrization of the sphere in terms of the usual polar angles,  $(\theta, \phi) \in [0, \pi] \times [0, 2\pi)$ , is as follows:

$$\Omega : \begin{cases} g^1 &= \sin \theta \cos \phi, \\ g^2 &= \sin \theta \sin \phi, \\ g^3 &= \cos \theta. \end{cases} \quad (4)$$

The corresponding measure is abbreviated by  $dg = \sin \theta d\theta d\phi$ .

We consider a higher order DTI representation of the form

$$D(g) = \sum_{k=0}^{\infty} D^{i_1 \dots i_k} g_{i_1} \dots g_{i_k}. \quad (5)$$

(Under the stipulated symmetry,  $D(g) = D(-g)$ , only even orders will be of interest.) The collection of polynomials on the sphere,

$$\mathcal{B} = \bigcup_{k \in \mathbb{N} \cup \{0\}} \mathcal{B}_k, \quad (6)$$

spanned by the monomial subsets

$$\mathcal{B}_k = \{g_{i_1} \dots g_{i_k} \mid k \in \mathbb{N} \cup \{0\} \text{ fixed}\}, \quad (7)$$

is complete, but redundant. Apart from the fact that odd order monomials are of no interest, redundancy is evident from the fact that lower order even monomials can be reproduced from higher order ones through contractions as a consequence of the quadratic constraint that defines the embedded unit sphere, recall Eq. (2). As a result, we have, e.g.,

$$g_{i_1} \dots g_{i_k} = \eta^{i_{k+1} i_{k+2}} g_{i_1} \dots g_{i_{k+2}}, \quad (8)$$

<sup>1</sup>The covector model reflects the physical nature of the components as normalized diffusion sensitizing gradients, i.e. covectors.

and, by recursion, we find similar dependencies for all lower order monomials in terms of higher order ones. Thus any monomial of order  $k \leq N \in \mathbb{N} \cup \{0\}$  is linearly dependent on the set of  $N$ -th order monomials of equal (even/odd) parity. This, of course, justifies the approach by Özarlan and Mareci [Özarlan and Mareci 2003], in which the data are fitted only against linear combinations of  $N$ -th order monomials, discarding all lower order terms. In particular, the larger  $N$  is, the better the approximation of the data will be. However, in the process of updating  $N$ , all HARDI data information will migrate to the tensor coefficients of corresponding rank. The reader is referred to the seminal paper by Özarlan and Mareci [Özarlan and Mareci 2003] for further details and physical background.

Still, it is not necessary to employ a basis of fixed order monomials. One can actually exploit the redundancy in  $\mathcal{B}$ , Eq. (6). For instance, we have

$$\mathcal{F}_N = \binom{N+2}{N} \quad (9)$$

independent  $N$ -th order basis monomials due to symmetry, as opposed to  $N!$  for an arbitrary rank- $N$  tensor. It also follows that  $\mathcal{F}_N$  is in fact the exact number of degrees of freedom of our full  $N$ -th order polynomial expansion, i.e. including all monomials of orders less than  $N$ . Consequently, if we retain all lower order monomials, it follows from Eq. (8) that the *effective* number of independent degrees of freedom in our  $N$ -th order term must be lower than  $\mathcal{F}_N$ , recall Eq. (9), viz. equal to the number of independent components of the symmetric rank- $N$  tensor minus the number of degrees of freedom already contained in the lower order terms:

$$\mathcal{F}_N^{\text{residual}} = \mathcal{F}_N - \mathcal{F}_{N-2} = 2N + 1. \quad (10)$$

This number therefore corresponds to the dimensionality of the residual degrees of freedom. If, in case of even  $N$ , we count all spherical harmonics  $Y_\ell^m$  for even  $\ell = N, N-2, \dots, 0$ , and all  $m \in \{-\ell, \dots, \ell\}$ —let us call this number  $\mathcal{G}_N$ —then we reobtain Eq. (9), since

$$\mathcal{G}_N = \sum_{\ell=0, \ell \text{ even}}^N (2\ell + 1) = \frac{(N+1)(N+2)}{2} = \mathcal{F}_N. \quad (11)$$

(The same result holds for  $N$  odd, in which case summation should be restricted to odd  $\ell$ -values only, but this is not relevant for us.) Notice that, in particular, the number of independent degrees of freedom of the spherical harmonics of order  $N$ ,  $\mathcal{G}_N^{\text{residual}}$  say, likewise equals

$$\mathcal{G}_N^{\text{residual}} = \mathcal{G}_N - \mathcal{G}_{N-2} = 2N + 1 = \mathcal{F}_N^{\text{residual}}. \quad (12)$$

These counting arguments suggest an intimate relationship between the rank- $k$  tensor coefficients of Eq. (5) in our scheme, v.i., and the spherical harmonics of order  $k$ .

Model redundancy may be beneficial, to the extent that it enables us to distribute the HARDI degrees of freedom *hierarchically* over the various orders involved, in such a way that only residual information is encoded in the higher order tensor coefficients. As  $N \rightarrow \infty$  this residual tends to zero, while all established tensor coefficients of lower rank than  $N$  remain fixed in the process of incrementing  $N$ . (The hierarchy implicit in Özarlan and Mareci's scheme is of a different nature.) We return to the potential benefit of our inhomogeneous polynomial expansion below.

We construct the coefficients as follows. Suppose we are in possession of  $D^{i_1 \dots i_k}$  for all  $k = 0, \dots, N-1$ , then we consider the

function

$$E_N(D^{j_1 \dots j_N}) = \int \left( D(g) - \sum_{k=0}^N D^{i_1 \dots i_k} g_{i_1} \dots g_{i_k} \right)^2 dg, \quad (13)$$

and find the  $N$ -th order coefficients by minimization. Setting

$$\frac{\partial E_N(D^{j_1 \dots j_N})}{\partial D^{i_1 \dots i_N}} = 0, \quad (14)$$

one obtains the following linear system:

$$\Gamma_{i_1 \dots i_N j_1 \dots j_N} D^{j_1 \dots j_N} = \int D(g) g_{i_1} \dots g_{i_N} dg - \sum_{k=0}^{N-1} \Gamma_{i_1 \dots i_N j_1 \dots j_k} D^{j_1 \dots j_k}, \quad (15)$$

with symmetric covariant tensor coefficients

$$\Gamma_{i_1 \dots i_k} = \int g_{i_1} \dots g_{i_k} dg. \quad (16)$$

The appearance of the second inhomogeneous term on the r.h.s. of Eq. (15), absent in the scheme proposed by Özarşlan and Mareci, reflects the fact that in our scheme higher order coefficients encode residual information only.

It is immediately evident that

$$\Gamma_{i_1 \dots i_{2k+1}} = 0 \quad (k \in \mathbb{N} \cup \{0\}), \quad (17)$$

since no odd-rank tensors with covariantly constant coefficients exist. All even-rank tensors of this type must be products of the Euclidean metric tensor, so we stipulate

$$\Gamma_{i_1 \dots i_{2k}} = \gamma_k \eta_{(i_1 i_2} \dots \eta_{i_{2k-1} i_{2k})}, \quad (18)$$

for some constant  $\gamma_k$ . Parentheses denote index symmetrization. The constant  $\gamma_k$  needs to be determined for each  $k \in \mathbb{N} \cup \{0\}$ .

One way to determine  $\gamma_k$  is to perform a full contraction of indices in Eq. (18), which, with the help of Eqs. (2) and (16), yields

$$\gamma_k = \frac{\Gamma}{\eta_{(i_1 i_2} \dots \eta_{i_{2k-1} i_{2k})} \eta^{i_1 i_2} \dots \eta^{i_{2k-1} i_{2k}}}. \quad (19)$$

To find the denominator on the r.h.s. is an exercise in combinatorics [Grimaldi 1993], and requires the basic trace property  $\eta_{ij} \eta^{ij} = \delta_i^i = n$ . A simpler way to find  $\gamma_k$  is to evaluate Eq. (18) for  $i_1 = \dots = i_{2k} = 1$  in a Cartesian coordinate system, since the symmetric product of metric tensors on the r.h.s. evaluates to 1 for this case:

$$\gamma_k = \Gamma_{1 \dots \leftarrow 2k \text{ indices} \rightarrow \dots 1} = \int g_1^{2k} dg. \quad (20)$$

This integral is a special case of the closed-form multi-index representation of Eq. (16), cf. Folland [Folland 2001] and Johnston [Johnston 1960], viz.:

$$\int g_1^{\alpha_1} \dots g_n^{\alpha_n} dg = \frac{2}{\Gamma(\frac{1}{2}|\alpha| + \frac{n}{2})} \prod_{i=1}^n \Gamma(\frac{1}{2}\alpha_i + \frac{1}{2}), \quad (21)$$

if all  $\alpha_j$  are even (otherwise the integral vanishes). Here  $|\alpha| = \alpha_1 + \dots + \alpha_n = 2k$  denotes the norm of the multi-index, and

$$\Gamma(t) = \int_0^\infty s^{t-1} e^{-s} ds = 2 \int_0^\infty r^{2t-1} e^{-r^2} dr \quad (22)$$

is the gamma function. Recall  $\Gamma(\ell) = (\ell - 1)!$  and  $\Gamma(\ell + \frac{1}{2}) = (\ell - \frac{1}{2}) \dots \frac{1}{2} \sqrt{\pi} = (2\ell)! \sqrt{\pi} / (4^\ell \ell!)$  for non-negative integers  $\ell \in \mathbb{N} \cup \{0\}$ . For the specific monomial in Eq. (20) we have  $\alpha = (2k, 0, \dots, 0) \in \mathbb{Z}^n$ .

**Result 1** Recall Eqs. (16–18). For general  $n$  we have

$$\gamma_k = \frac{2\Gamma(k + \frac{1}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(k + \frac{n}{2})},$$

in other words,

$$\Gamma_{i_1 \dots i_{2k}} = \frac{2\Gamma(k + \frac{1}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(k + \frac{n}{2})} \eta_{(i_1 i_2} \dots \eta_{i_{2k-1} i_{2k})}.$$

For  $n = 3$  in particular, we obtain

$$\gamma_k = \frac{2\pi}{k + \frac{1}{2}},$$

whence

$$\Gamma_{i_1 \dots i_{2k}} = \frac{2\pi}{k + \frac{1}{2}} \eta_{(i_1 i_2} \dots \eta_{i_{2k-1} i_{2k})}.$$

This result is the tensorial counterpart of Eq. (21). Some examples ( $n = 3$ ):

$$\begin{aligned} k = 0 & : \Gamma & = & 4\pi \\ k = 1 & : \Gamma_{ij} & = & \frac{4\pi}{3} \eta_{ij} \\ k = 2 & : \Gamma_{ijkl} & = & \frac{4\pi}{15} (\eta_{ij} \eta_{kl} + \eta_{ik} \eta_{jl} + \eta_{il} \eta_{jk}). \end{aligned}$$

The corresponding linear systems, recall Eq. (15), are as follows:

$$\begin{aligned} \Gamma D & = \int D(g) dg, \\ \Gamma_{ij} D^j & = \int D(g) g_i dg - \Gamma_i D, \\ \Gamma_{ijkl} D^{kl} & = \int D(g) g_i g_j dg - \Gamma_{ij} D - \Gamma_{ijk} D^k. \end{aligned}$$

It follows that the scalar constant  $D$  is just the average diffusivity over the unit sphere:

$$D = \frac{\int D(g) dg}{\int dg}. \quad (23)$$

The constant vector  $D^i$  vanishes identically, as it should. For the rank-2 tensor coefficients we find the traceless matrix

$$D_{ij} = \frac{15 \int D(g) g_i g_j dg - 5 \int D(g) dg \eta_{ij}}{2 \int dg}, \quad (24)$$

and so forth. If, instead, we fit a homogeneous second order polynomial to the data (by formally omitting the second term on the r.h.s. of Eq. (15)), as proposed by Özarşlan and Mareci, we obtain the following rank-2 tensor coefficients:

$$D_{ij}^{\text{ö.m.}} = \frac{15 \int D(g) g_i g_j dg - 3 \int D(g) dg \eta_{ij}}{2 \int dg}, \quad (25)$$

which is clearly different. However, Özarşlan and Mareci's homogeneous polynomial expansion should be compared to our inhomogeneous expansion. Indeed, if we compare the respective second order expansions in this way we observe that  $D_2^{\text{ö.m.}}(g) = D_2(g)$ . The difference in coefficients, in this example, is explained by the contribution already contained in the lowest order term of our polynomial, which in Özarşlan and Mareci's scheme has to migrate to the second order tensor.

In general we raise the conjecture that to any order  $N$  we have equality.

**Theorem 1** Let  $D_N(g)$  denote the truncated expansion of Eq. (5) including monomials of orders  $k \leq N$  only, and let  $D_N^{\hat{O},M}(g)$  denote the  $N$ -th order homogeneous polynomial expansion proposed by Özarlan and Mareci, loc. cit., then

$$D_N^{\hat{O},M}(g) = D_N(g).$$

However, the interesting claim we wish to make is the following, which shows exactly what we mean by the hierarchical ordering of degrees of freedom in our inhomogeneous expansion:

**Theorem 2** If  $\Delta$  denotes the Laplace-Beltrami operator on the unit sphere, then for any  $N \in \mathbb{N} \cup \{0, \infty\}$

$$D_N(g, t) \equiv e^{t\Delta} D_N(g) = \sum_{k=0}^N D^{i_1 \dots i_k}(t) g_{i_1} \dots g_{i_k},$$

with

$$D^{i_1 \dots i_k}(t) = e^{-k(k+1)t} D^{i_1 \dots i_k}.$$

For brevity we set  $D(g, t) = D_\infty(g, t)$ .

This is nontrivial, since the monomials  $g_{i_1} \dots g_{i_n}$  are themselves not eigenfunctions of the Laplace-Beltrami operator. The construction of the coefficients in the linear combinations as they occur in the inhomogeneous expansion, implicitly defined by Eq. (15), is apparently crucial. For instance, the scaling of the second order term in Theorem 2 is a direct consequence of the fact that the coefficient matrix in Eq. (24) is traceless, as opposed to Eq. (25).

**Proof of Theorems 1–2.** Consider the following closed linear subspace of  $L_2(\Omega)$  for even  $N$ :

$$X_N = \text{span} \{g_{i_1} \dots g_{i_N}\} = \bigoplus_{k=0}^{N/2} S_{2k},$$

in which  $S_{2k} = \text{span} \{Y_{2k}^m \mid m = -2k, -2k+1, \dots, 2k-1, 2k\}$ . Set  $\phi_N(g) = D(g) - D_{N-2}(g)$ , with induction hypothesis  $P_{S_{2k}} \phi_N = 0$  for all  $k = 0, \dots, N/2 - 1$ , in which  $P_{S_{2k}}$  denotes orthogonal projection onto  $S_{2k}$ . In other words, by hypothesis,

$$\phi_N \in \bigoplus_{k=N/2}^{\infty} S_{2k}.$$

Let  $\psi_N \in X_N$  be such as to minimize  $E(\psi) = \|\phi_N - \psi\|_{L_2(\Omega)}$  for  $\psi \in X_N$ . Obviously  $P_{S_N} \phi_N \in X_N$ , so that by definition of  $\psi_N$  we obtain

$$\|\phi_N - \psi_N\|_{L_2(\Omega)} \leq \|\phi_N - P_{S_N} \phi_N\|_{L_2(\Omega)}.$$

On the other hand, since  $\phi_N - P_{S_N} \phi_N \perp P_{S_N} \phi_N - \psi_N$ , we also have

$$\begin{aligned} \|\phi_N - \psi_N\|_{L_2(\Omega)}^2 &= \|\phi_N - P_{S_N} \phi_N + P_{S_N} \phi_N - \psi_N\|_{L_2(\Omega)}^2 = \\ &= \|\phi_N - P_{S_N} \phi_N\|_{L_2(\Omega)}^2 + \|P_{S_N} \phi_N - \psi_N\|_{L_2(\Omega)}^2 \\ &\geq \|\phi_N - P_{S_N} \phi_N\|_{L_2(\Omega)}^2. \end{aligned}$$

We conclude that

$$\|\phi_N - \psi_N\|_{L_2(\Omega)} = \|\phi_N - P_{S_N} \phi_N\|_{L_2(\Omega)},$$

in other words,  $\psi_N = P_{S_N} \phi_N$ , so that apparently  $\psi_N \in S_N$ . Note that  $S_k$  is precisely the degenerate eigenspace of the Laplace-Beltrami operator,  $\Delta$ , with corresponding eigenvalue  $-k(k+1)$ , whence the eigenvalue of  $\exp(t\Delta)$  equals  $\exp(-k(k+1)t)$ . This completes the proof.  $\square$

The significance of Theorem 2 is that it segregates degrees of freedom in the polynomial expansion in such a way that we may interpret each homogeneous higher order term as an incremental refinement of detail relative to that of the lower order expansion. To see this, note that  $D_N(g, t)$  satisfies the heat equation on the unit sphere, recall Eq. (3):

$$\frac{\partial u}{\partial t} = \frac{1}{\sqrt{g}} \partial_\mu (g^{\mu\nu} \sqrt{g} \partial_\nu u) = \Delta u, \quad (26)$$

in which the initial condition corresponds to the  $N$ -th order expansion of the raw data,  $D_N(g, 0) = D_N(g)$ . Recall that in the usual polar coordinates in  $n = 3$  dimensions we have for a scalar function on the unit sphere:

$$\Delta u(\theta, \phi) = \left( \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right) u(\theta, \phi). \quad (27)$$

The remarkable fact is thus that the linear combinations  $D^{i_1 \dots i_k} g_{i_1} \dots g_{i_k}$ , unlike the monomials  $g_{i_1} \dots g_{i_k}$  separately, are eigenfunctions of the heat operator  $\exp(t\Delta)$ , i.e. *self-similar polynomials on the sphere*, which admit a reformulation in terms of purely  $k$ -th order spherical harmonics, with eigenvalues  $e^{-k(k+1)t}$ . The heat operator can be seen as the canonical resolution degrading semigroup operator [Koenderink 1984; Florack 1997]. The parameter  $t$  denotes the (square of) angular scale, or inverse resolution, at which the raw data are resolved. Indeed, the classical rank-2 DTI representation, defined via the Stejskal-Tanner formula [Özarlan and Mareci 2003; Stejskal and Tanner 1965]:

$$S(g) = S_0 \exp(-bD(g)), \quad (28)$$

arises not merely as an approximation under the assumption that the diffusion attenuation can be written as

$$D(g) \approx D_{\text{DTI}}(g) = D_{\text{DTI}}^{ij} g_i g_j, \quad (29)$$

but expresses the *exact* asymptotic behaviour of  $D(g, t)$  as  $t \rightarrow \infty$ , recall Eq. (2) and Theorem 2:

$$D(g, t) = \underbrace{\left( D \eta^{ij} + e^{-6t} D^{ij} \right)}_{D_{\text{DTI}}(g, t) = D_{\text{DTI}}^{ij}(t) g_i g_j} g_i g_j + \mathcal{O}(e^{-12t}) \quad (t \rightarrow \infty). \quad (30)$$

It shows that the DTI tensor is not self-similar, but has a bimodal resolution dependence. The actual limit of truly vanishing resolution is of course given by a complete averaging over the sphere:

$$\lim_{t \rightarrow \infty} D(g, t) = \lim_{t \rightarrow \infty} D_{\text{DTI}}(g, t) = D, \quad (31)$$

recall Eq. (23). See Figs. 1–2 for an illustration of Theorem 2 for  $N = 8$  on a synthetic image with Rician noise.

### 3 Conclusion

We have proposed a tensorial representation of high angular resolution diffusion images (HARDI), or derived functions defined on the unit sphere, in terms of a family of inhomogeneous polynomials on the sphere. The resulting polynomial representation, truncated at some arbitrary order, or formally extended into an infinite series, may be regarded as the canonical way of decomposing HARDI data into “higher order diffusion tensors”, to the extent that the successive homogeneous terms capture residual information only, i.e. degrees of freedom that cannot be detailed by a lower order expansion. In this sense they form the tensorial counterpart of the spherical harmonic decomposition. A related consequence is that the inhomogeneous polynomial expansion neatly segregates the HARDI signal

into a hierarchy of homogeneous polynomials that are *self-similar* under the act of graceful resolution degradation induced by heat operator,  $\exp(t\Delta)$ , generated by the isotropic Laplace-Beltrami operator  $\Delta$  on the sphere, with a characteristic decay that depends on order (for fixed  $t \in \mathbb{R}^+$ ). The asymptotic case of almost vanishing resolution ( $t \rightarrow \infty$ ) reproduces the diffusion tensor of classical diffusion tensor imaging (DTI), with one constant and one resolution-dependent mode. The true asymptotic case leads to a complete averaging over the sphere, as expected. The general  $N$ -th order expansion provides control over the trade-off between regularity (choice of  $t$ ) and complexity (choice of  $N$ ), i.e. descriptive power. Finally, we have related our result to the homogeneous polynomial expansion proposed by Özarslan and Mareci [Özarslan and Mareci 2003], and argued that the expansions lead to identical results despite the differences in coefficients. We have stressed the fact that this is possible by virtue of the redundancy inherent in the use of an inhomogeneous polynomial representation.

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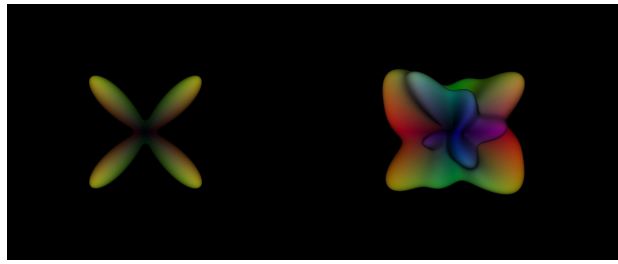


Figure 1: Left: Synthetic noise-free profile induced by two crossing fibers at right angle. Right: Same, but with Rician noise.

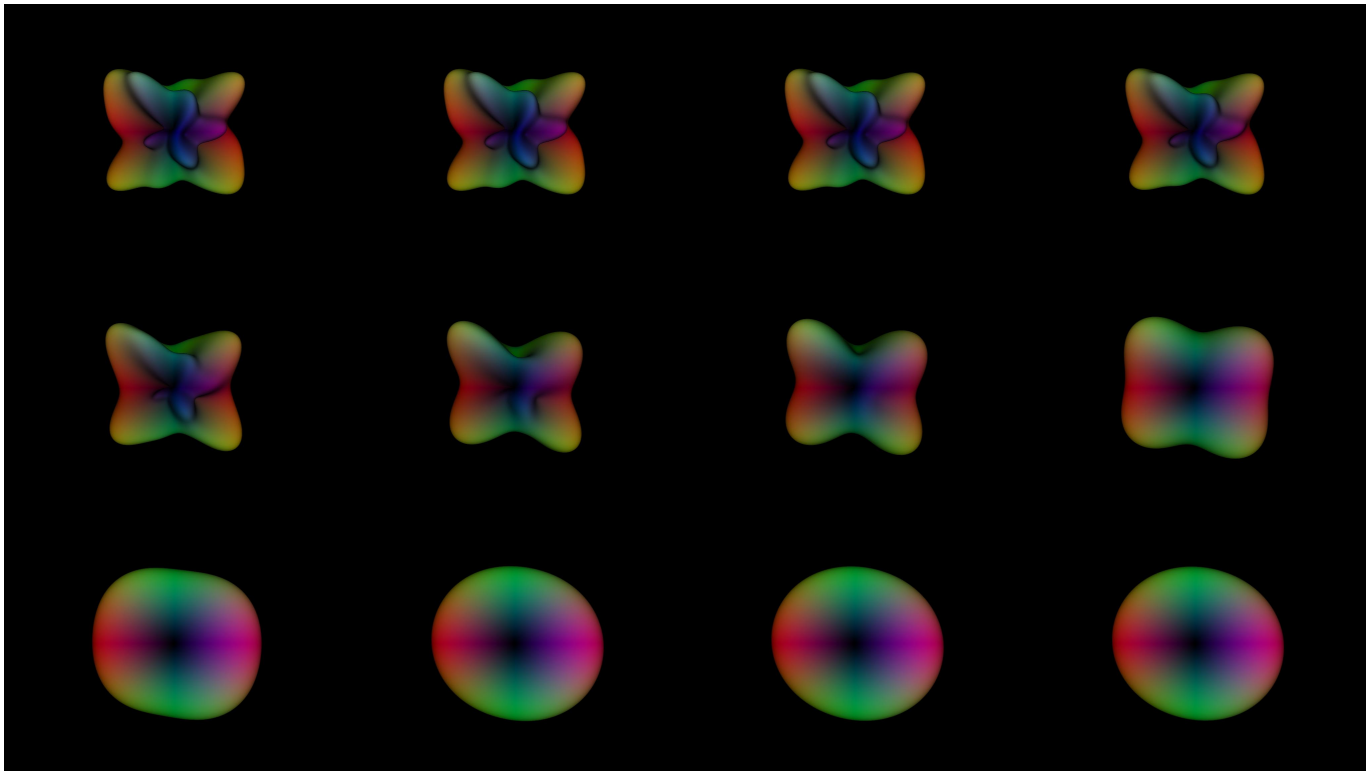


Figure 2: Regularized profiles produced from the right image in Fig. 1 using Theorem 2 for  $N = 8$ . The regularization parameter  $t$  increases exponentially from top left to bottom right over the range 0.007–1.0.