COMPUTATIONAL HARMONIC ANALYSIS FOR TENSOR FIELDS ON THE TWO-SPHERE

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Abstract. In this paper we describe algorithms for the numerical computation of Fourier transforms of tensor fields on the two-sphere, \( S^2 \). These algorithms reduce the computation of an expansion on tensor spherical harmonics to expansions in scalar spherical harmonics, and hence can take advantage of recent improvements in the efficiency of computation of scalar spherical harmonic transforms.

1. Introduction

The calculation of Fourier expansions for vector fields, and more generally, tensor fields on the two-sphere has been identified as an important computational problem in areas such as fluid dynamics [22] and global circulation modeling [61]. Other applications include the analysis of cosmic microwave background radiation [74] and models of stress propagation through the earth [24].

In this paper we show how the computation of expansions in tensor spherical harmonics may be reduced to a small number of scalar spherical harmonic transforms. Over the past twenty years a large body of work has grown, addressing the problem of efficient and stable computation of scalar spherical harmonic transforms [3, 52, 19, 32]. Our reduction of the tensor harmonic transform to scalar harmonic transforms allows this work to be applied to a new set of problems.

Our results generalize a well-known relationship between vector and scalar spherical harmonics (see, e.g., [48]) to the case of tensor spherical harmonics. This relation was used for analysis of shallow water models by C. Temperton [64] to reduce the computation of vector harmonics to that of scalar harmonics. Thus, our work can be considered a generalization of Temperton’s \( u,v \) approach to phenomena that are described by tensor fields.

To verify that our results give a practical method of computing tensor harmonic expansions, we implemented the algorithms and investigated their numerical accuracy experimentally. In the reduction to spherical harmonics some issues of numerical stability do arise, and these are examined. The reduction to spherical harmonic transforms is the main point of this paper, and in the subsequent computation of the transforms, any accurate routine for computing the scalar harmonic transform can be used. For convenience we chose a method based on the so-called “semi-naive” algorithm [18, 20], a technique which computes the necessary discrete Legendre transforms in the frequency domain.

The organization of the paper is as follows. We start in Section 2 with a brief overview of the theory of vector and scalar harmonics. In Section 3 we discuss the tensor spherical harmonics introduced by Newman and Penrose [50], and develop the properties needed to relate these to scalar spherical harmonics. These tensor harmonics are also known as monopole harmonics.

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[72, 73], and are the natural choice for the expansion of tensor fields on the sphere. In Section 4 we develop a sampling theory for tensor fields on the sphere in both the band-limited, and non-band-limited settings. In Section 5 we combine the sampling and tensor harmonic results to get explicit algorithms for computing the expansion of a finitely sampled tensor field in terms of tensor harmonics. We present our numerical results in Section 6, and conclude in Section 7.

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2. Harmonic analysis on the two-dimensional sphere

Since the scalar spherical transform will play a pivotal role in our development of tensor spherical transforms, we first provide a brief review of scalar spherical harmonics. We emphasize their relation to the Laplacian operator and rotation invariance, as these will be the defining properties that we generalize for defining tensor harmonics.

Rotationally invariant differential operators occur throughout the physical sciences. It is a well-known fact that any such operator may be expressed as a sum of powers of the Laplacian, here denoted as $\Delta$. In coordinates, $\Delta$ is defined by

\[
\Delta = -\left(\frac{\partial^2}{\partial \varphi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}\right),
\]

where $\theta$ is the co-latitude, and $\varphi$ is the azimuthal coordinate (cf. Figure 1).

0 $\leq \theta \leq \pi$
0 $\leq \varphi < 2\pi$

**Figure 1.** Co-latitude and azimuthal coordinates.

The spherical harmonics are an orthogonal system of functions on the two-dimensional sphere that diagonalize any rotationally invariant differential operator. This accounts for their ubiquity in problems involving spherical symmetry. In terms of the Laplacian, the spherical harmonics are defined up to a scalar multiple by the properties

\[
\Delta Y_{lm} = l(l + 1)Y_{lm} \quad \text{and} \quad \frac{1}{i} \frac{\partial Y_{lm}}{\partial \varphi} = mY_{lm}.
\]

These conditions imply that $l$ and $m$ are integers with $|m| \leq l$.

Mathematicians and physicists use a number of different conventions for the normalization of the spherical harmonics. We normalize things so that the expression for $Y_{lm}$ in coordinates becomes

\[
Y_{lm}(\theta, \varphi) = P_l^m(\cos \theta)e^{im\varphi},
\]
where $P_m$ is the associated Legendre function defined by

$$P_m(x) = \frac{1}{2^m m!} \frac{d^m}{dx^m} \left( 1 - x^2 \right)^{m/2}.$$

With this normalization, the spherical harmonics satisfy the additional symmetry under complex conjugation, $\bar{Y}_{lm} = Y_{l,-m}$, and have $L^2$-norm

$$||Y_{lm}||_2^2 = \int_0^\pi \int_0^{2\pi} |Y_{lm}(\theta, \varphi)|^2 \sin \theta d\theta d\varphi = \frac{4\pi}{2l+1} \frac{(l+m)!}{(l-m)!}.$$

The spherical harmonics are orthogonal with respect to the inner product

$$\langle f, h \rangle = \int_0^\pi \int_0^{2\pi} f(\theta, \varphi) \overline{h(\theta, \varphi)} \sin \theta d\theta d\varphi.$$

Using this inner product, any square-integrable function on the sphere may be expanded in the spherical harmonic basis. The formula for the expansion is

$$f = \sum_{|m| \leq l} ||Y_{lm}||_2^{-2} \hat{f}(l, m) \cdot Y_{lm},$$

where the sum converges in the mean, and the coefficients $\hat{f}(l, m)$ are defined by $\hat{f}(l, m) = \langle f, Y_{lm} \rangle$. The function $\hat{f}(l, m)$ is called the spherical harmonic transform of $f$, and as the formulas (3) and (6) for spherical harmonics and inner products show, it may be computed using a Fourier transform on the azimuthal variable $\varphi$ followed by integration over the colatitude $\theta$.

### 2.1. Vector Spherical Harmonics

So far we have only considered the expansion of a complex scalar function on the sphere in terms of an orthogonal basis of scalar functions, the spherical harmonics. This basis was determined, up to normalization constants, by its properties under rotations of the sphere (cf. (2)) and a choice of a distinguished point (and hence an axis) on the sphere, the north pole.

There is an analogous expansion for vector fields on the sphere. We shall define an inner product on the space of such vector fields and choose a basis for the resulting Hilbert space, the vector spherical harmonics, based on a set of specified properties under rotation, and in this way generalize the construction of the scalar spherical harmonics. Consequently, in the same way that scalar spherical harmonics are used in spectral method approaches for numerical solution of scalar PDEs or data analysis of scalar data on the sphere, the vector spherical harmonics may be used effectively in cases where the data consists of vector fields on the sphere. Typical examples that arise in practice are electromagnetic fields or wind velocity.

We start our analysis by noting that we need only consider tangential vector fields on the sphere. If we consider the sphere as embedded in 3-space, then it is natural to view any vector field as the direct sum of a purely radial field and an orthogonal tangential field. The purely radial vector fields transform under rotations in exactly the same way as scalar fields, and so the appropriate basis for the subspace of purely radial vector fields consists of the fields of the form $Y_{lm} e_r$, where $e_r$ is the radial vector field of unit vectors. Hence, radial vector fields may be treated using the methods developed for scalar spherical harmonics. The complementary space of vector fields, the tangential vector fields, requires a separate treatment.

Any tangential vector field on the sphere can be expressed, except at the poles, in terms of the usual unit vector fields $e_\theta$ and $e_\varphi$ which are generated by polar coordinates $(\theta, \varphi)$ [61]. I.e., any real tangential vector field $\mathbf{v}$ may be written as

$$\mathbf{v} = v_\theta e_\theta + v_\varphi e_\varphi.$$
where \( v_\theta \) and \( v_\varphi \) are real-valued functions defined on \( S^2 \) except at the poles. For our purposes it is most convenient, though not essential, to work with complex vector fields, in which case the functions \( v_\theta \) and \( v_\varphi \) are complex-valued. Given two tangential vector fields \( \mathbf{u} \), and \( \mathbf{v} \), define their inner product to be

\[
\langle \mathbf{u}, \mathbf{v} \rangle = \int_{S^2} u_\theta v_\theta^* + u_\varphi v_\varphi^* \, d\mu
\]

where \( d\mu = \sin \theta \, d\theta \, d\varphi \) is the invariant measure on the sphere; we denote the corresponding Hilbert space by \( L^2(S^2) \).

In order to generalize the eigenvalue equations (2), we must generalize the Laplacian and angular momentum operators to act on tangential vector fields. The Laplacian of the vector field \( \mathbf{v} = v_\theta \mathbf{e}_\theta + v_\varphi \mathbf{e}_\varphi \) can be defined using the Riemannian metric on the sphere, or as the image of the Casimir operator under the action of the rotation group. In either case, the formula in coordinates is

\[
\Delta \mathbf{v} = \left[ -\left( \frac{\partial^2}{\partial \theta^2} + \frac{\cot \theta}{\sin^2 \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} - \frac{1}{\sin^2 \theta} \right) v_\theta + \frac{2 \cot \theta}{\sin \theta} \frac{\partial v_\varphi}{\partial \varphi} \right] \mathbf{e}_\theta + \left[ -\left( \frac{\partial^2}{\partial \varphi^2} + \frac{\cot \theta}{\sin^2 \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} - \frac{1}{\sin^2 \theta} \right) v_\varphi - \frac{2 \cot \theta}{\sin \theta} \frac{\partial v_\theta}{\partial \varphi} \right] \mathbf{e}_\varphi.
\]

The angular momentum operator is defined by

\[
J_z \mathbf{v} = \frac{1}{i} \frac{\partial v_\theta}{\partial \varphi} \mathbf{e}_\theta + \frac{1}{i} \frac{\partial v_\varphi}{\partial \varphi} \mathbf{e}_\varphi
\]

and is the infinitesimal generator for rotations around the \( z \)-axis.

The vector spherical harmonics, \( \mathbf{B}_{lm} \), and \( \mathbf{C}_{lm} \), are defined so that they satisfy the differential equations

\[
\Delta \mathbf{B}_{lm} = \ell(\ell + 1) \mathbf{B}_{lm} \quad \text{and} \quad J_z \mathbf{B}_{lm} = m \mathbf{B}_{lm},
\]

\[
\Delta \mathbf{C}_{lm} = \ell(\ell + 1) \mathbf{C}_{lm} \quad \text{and} \quad J_z \mathbf{C}_{lm} = m \mathbf{C}_{lm}.
\]

The conditions (11) and (12) are analogous to the conditions (2) for the scalar spherical harmonics, but unlike the scalar case, these equations have a two-dimensional space of solutions for each \( \ell \) and \( m \) with \( \ell \geq 1 \) and \( |m| \leq \ell \), giving rise to two independent vector spherical harmonics, \( \mathbf{B}_{lm} \) and \( \mathbf{C}_{lm} \).

Following Morse and Feshbach [48], if we define

\[
\mathbf{B}_{lm} = \frac{1}{\sqrt{l(l+1)}} \left[ \frac{\partial Y_{lm}}{\partial \theta} \mathbf{e}_\theta + \frac{1}{\sin \theta} \frac{\partial Y_{lm}}{\partial \varphi} \mathbf{e}_\varphi \right]
\]

and

\[
\mathbf{C}_{lm} = -\mathbf{e}_\times \mathbf{B}_{lm}
\]

then \( \mathbf{B}_{lm} \) and \( \mathbf{C}_{lm} \) each satisfy the eigenvalue equations (11) and (12). The collection of vector fields \( \{ \mathbf{B}_{lm}, \mathbf{C}_{lm} \} \) for \( 1 \leq \ell \) and \( |m| \leq \ell \), forms a complete basis of orthogonal vector fields in the space of all tangential vector fields, with normalization constants the same as for the scalar spherical harmonics, i.e.,

\[
||\mathbf{B}_{lm}||^2 = ||\mathbf{C}_{lm}||^2 = ||Y_{lm}||^2 = \frac{4\pi}{2\ell + 1} \frac{(l+m)!}{(l-m)!}.
\]
Hence any vector field on the sphere may be written as
\[ \mathbf{v} = \sum_{l \leq |m| \leq l} \frac{1}{\sqrt{l(l+1)}} \left[ f^B(l, m) \mathbf{B}_m + f^C(l, m) \mathbf{C}_m \right] \]
where \( f^B(l, m) = \langle \mathbf{v}, \mathbf{B}_m \rangle \), and \( f^C(l, m) = \langle \mathbf{v}, \mathbf{C}_m \rangle \). The map from the vector field \( \mathbf{v} \) to the coefficients \( \{ f^B(l, m), f^C(l, m) \} \) is called the vector harmonic transform.

To relate the vector harmonic transform to the scalar harmonic transform, simply note that
\[ \mathbf{B}_m = \frac{1}{\sqrt{l(l+1) \sin \theta}} \left[ \frac{1}{2l+1} [l(l-m+1)Y_{l+1,m} - (l+1)(l+m)Y_{l-1,m}] \mathbf{e}_\theta + i m Y_{l,m} \mathbf{e}_\varphi \right] \]
and
\[ \mathbf{C}_m = \frac{1}{\sqrt{l(l+1) \sin \theta}} \left[ \frac{1}{2l+1} [l(l-m+1)Y_{l+1,m} - (l+1)(l+m)Y_{l-1,m}] \mathbf{e}_\varphi \right]. \]

Hence, if we define auxiliary quantities \( g^\theta(l, m) \) and \( g^\varphi(l, m) \) by
\[ g^\theta(l, m) = \langle \frac{1}{\sin \theta} \mathbf{v}_\theta, Y_{l,m} \rangle, \]
\[ g^\varphi(l, m) = \langle \frac{1}{\sin \theta} \mathbf{v}_\varphi, Y_{l,m} \rangle \]
then
\[ f^B(l, m) = \frac{1}{\sqrt{l(l+1) \sin \theta}} \left[ \frac{1}{2l+1} g^\theta(l+1, m) - \frac{(l+1)(l+m)}{2l+1} g^\theta(l-1, m) \right] \]
\[ f^C(l, m) = \frac{1}{\sqrt{l(l+1) \sin \theta}} \left[ -ig^\varphi(l, m) - \frac{l(l-m+1)}{2l+1} g^\varphi(l+1, m) + \frac{(l+1)(l+m)}{2l+1} g^\varphi(l-1, m) \right]. \]

Equations (15) and (16) allow us to compute a vector harmonic transform by means of two scalar transforms. Once we have calculated the quantities \( g^\theta(l, m) \) and \( g^\varphi(l, m) \) for \( l \geq 1 \) and \( |m| \leq l \leq N + 1 \) (this will be discussed in section 3), we may use equations (15) and (16) to calculate \( f^B(l, m) \) and \( f^C(l, m) \) for \( 1, |m| \leq l \leq N \) in an additional \( 6((N+1)^2 - 1) \) scalar multiplications and \( 4((N+1)^2 - 1) \) scalar additions.

3. Harmonic analysis of tensor fields

3.1. The Spin-s Harmonics. There are several different definitions of tensor spherical harmonics which have been developed in the study of quantum mechanical angular momentum, gravitational radiation and group representations. The spin-s harmonics are an orthogonal basis of tensor fields that seems particularly well-suited to the harmonic analysis of tensor fields, of any rank, on the sphere. These tensor fields were introduced by Gel’fand, Minlos, and Shapiro [26], and were rediscovered by Newman and Penrose [50] who named them spin-s harmonics. Wu and Yang [72, 73] later defined equivalent versions of these tensor harmonics, calling them monopole harmonics. Our exposition follows the construction used in [50, 27].

The first step in our construction is to introduce a set of basis vectors and tensors at each point of the sphere apart from the poles. The fields \( \mathbf{e}_\theta \) and \( \mathbf{e}_\varphi \) are easily visualized, but are not the
most convenient fields to work with, because fields of the form \( v_b e_\theta \) or \( v_\varphi e_\varphi \) are not transformed onto fields of the same type under rotations. Define the fields \( e_+ \) and \( e_- \) by

\[
e_+ = \frac{1}{\sqrt{2}} (e_\theta - ie_\varphi), \quad e_- = \frac{1}{\sqrt{2}} (e_\theta + ie_\varphi).
\]

As with the fields \( e_\theta, e_\varphi \), the vectors \( e_+, e_- \) are orthonormal at each point of the sphere apart from the north and south poles. However, the set of fields of the form \( v_b e_\pm \) is invariant under rotations, and is also much better behaved at the poles; the lines generated by the vectors \( e_\pm \) converge to unique lines at each pole. I.e. the fields \( e_\pm \) are sections of homogeneous subbundles of the tangent bundle, away from the poles. Given a tangent vector field \( v \), we may write

\[
v = v_+ e_+ + v_- e_- , \quad \text{where} \quad v_\pm = \frac{1}{\sqrt{2}}(v_\theta \pm iv_\varphi).
\]

In this notation the inner product (8) can be rewritten as

\[
\langle u, v \rangle = \int_{S^2} u_+ \overline{v_+} + u_- \overline{v_-} \, d\mu.
\]

We denote the set of vector fields of the form \( v_\pm e_\pm \), by \( L^2(E_\pm) \).

Now construct fields of basis tensors generalizing \( e_+ \) and \( e_- \). Let \( e_0 = 1 \), and for \( n \geq 1 \) define

\[
e_n = e_+ \otimes \ldots \otimes e_+, \quad e_{-n} = e_- \otimes \ldots \otimes e_-.
\]

where the tensor products \( e_\pm \) have \( n \) factors. There is a natural identification \( e_\pm \otimes e_n = e_{n+m} \) for any integers \( n, m \), and we can use this identification to reduce the problem of finding harmonic expansions of arbitrary tensor fields on the sphere to the problem of expanding fields of the form \( f e_n \). A tensor field of the form \( f e_n \) is called a tensor field of type \( n \) or a tensor field with spin weight \( n \) [50]. Let \( L^2(E_n) \) denote the vector space of square integrable tensor fields of type \( n \), with the inner product

\[
\langle f e_n, g e_n \rangle = \int_{S^2} f \overline{g} \, d\mu.
\]

The definition of the tensor spherical harmonics is formally identical to the scalar harmonics, except that the Laplacian and angular momentum operators occurring in (2) are defined for tensor fields of type \( n \) instead of scalar fields. In coordinates, the Laplacian and angular momentum operators on tensor fields of type \( n \) are given by

\[
\Delta(f e_n) = - \left[ \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{2n \cot \theta}{\sin \theta} \frac{\partial}{\partial \varphi} - \frac{n^2}{\sin^2 \theta} \right) \right] f e_n
\]

and

\[
J_z(f e_n) = \left[ \frac{1}{i} \frac{\partial}{\partial \varphi} \right] f e_n.
\]

Then any invariant differential operator, from tensor fields of type \( n \) to tensor fields of type \( n \), is a sum of powers of the Laplacian, and the \( \text{spin-}n \) harmonics are defined up to a scalar multiple as solutions to the eigenvalue equations

\[
\Delta Y_{lm}^n = \ell(\ell + 1) Y_{lm}^n \quad \text{and} \quad J_z Y_{lm}^n = m Y_{lm}^n.
\]

To construct explicit formulæ for the \( \text{spin-}n \) harmonics, we use invariant differential operators between spaces of smooth tensor fields of different types. Define differential operators \( D_\pm \) from smooth tensor fields of type \( n \) to smooth tensor fields of type \( n \pm 1 \) by

\[
D_\pm(f e_n) = \left[ \left( \frac{\partial}{\partial \theta} \pm \frac{i}{\sin \theta} \frac{\partial}{\partial \varphi} \mp n \cot \theta \right) \right] f e_{n \pm 1}.
\]
Newman and Penrose [50] use the notation $\mathcal{O}^\pm$ for $D_+^\pm$ and $\mathcal{O}^\mp$ for $D_-^\mp$. We also define operators $D^\pm_n$ to be $D_\pm \cdots D_\pm (n \text{ factors})$ for $n > 0$.

**Remark.** Equation (18) defines differential operators acting on sections away from the north and south pole, but the differential operators extend smoothly to the entire sphere. This can be seen by looking at the action of $SO(2)$ on the universal enveloping algebra of $so(3)$. For any $p, n$, the space of differential operators from tensor fields of type $n$ to tensor fields of type $n + p$ is generated by $D_p^+$ both as a left module over the invariant differential operators on tensors of type $n + p$ and as a right module over the invariant differential operators on tensors of type $n$. A second way of constraining these generators is to project the covariant derivative onto sub-bundles of the tensor bundles of $S^2$.

Let

$$C_{nl} = \prod_{k=0}^{l|\Delta - 1} (l(l + 1) - k(k + 1)).$$

Then, the operators $D_\pm^\pm, D^\pm_n$ satisfy the following properties:

**Lemma 3.1.** (i) $D_\pm^\pm$ are rotationally invariant differential operators.

(ii) $D_\pm^\pm \Delta = \Delta D_\pm^\pm$ and $J_\pm D_\pm^\pm = D_\pm^\pm J_\pm$.

(iii) $D_\pm^\pm = -D_\mp^\pm$.

(iv) $D_\pm^\pm D_\mp^\pm = \Delta - n(n + 1)$ and $D_\pm^\pm D_\pm^\pm = \Delta - (n - 1)n$.

(v) $||D_nY_{lm}||^2 = C_{nl}||Y_{lm}||^2$

**Definition 3.1.** Define the monopole harmonics of type $n$, degree $l$ and order $m$ to be

$$Y_{lm}^n = \frac{1}{\sqrt{C_{nl}}} D_nY_{lm}e_0$$

We shall also call these the tensor spherical harmonics.

Equations (17) and (19) now imply that the the functions $Y_{lm}^n$ make up a basis for $L^2(E_n)$.

**Theorem 3.2.** The set of functions $\{Y_{lm}^n : |n| \leq l, |m| \leq l\}$, defined in (17) is an orthogonal basis for $L^2(E_n)$, satisfying (17), and such that $||Y_{lm}^n||^2 = ||Y_{lm}||^2$. Any such basis for $L^2(E_n)$ is uniquely determined up to phase factors.

Thus, by Theorem 3.2 any tensor field, $v = fe_n$ of type $n$ has an expansion

$$v = \sum_{|n|, |m| \leq l} \frac{1}{||Y_{lm}||^2} f_{lm}^n Y_{lm}^n$$

where

$$f_{lm}^n = \langle v, Y_{lm}^n \rangle = \int_{S^2} f \cdot X_{lm}^n \, d\mu$$

and $X_{lm}^n$ is a function on $S^2$ such that $Y_{lm}^n = X_{lm}^n e_n$. The function $f_{lm}^n$ is called the tensor harmonic transform of the tensor field $f$.

**Example 3.3.** The spin-1 and spin-\((-1)\) harmonics are simply related to the vector spherical harmonics of [48] through the equations

$$B_{lm} = \frac{1}{\sqrt{2}} [Y_{lm}^{-1} + iY_{lm}^1]$$

$$C_{lm} = -\frac{1}{\sqrt{2}} [iY_{lm}^1 + Y_{lm}^{-1}]$$
The fields $B_m, C_m$ have the advantage of being real, at a cost of poorer invariance properties.

Just as in the case of vector spherical harmonics, our definition of the tensor harmonics (Definition 3.1) is given in terms of derivatives of the scalar spherical harmonics, but for computational purposes we may require a more explicit definition in terms of linear combinations of products of trigonometric functions and scalar harmonics, i.e., we would like an expression for the $X_{l,m}^n$. To this end, define the differential operator

$$B = \frac{\partial}{\partial \theta} + \frac{i}{\sin \theta} \frac{\partial}{\partial \phi}.$$  

and let $B_0 = B$ and then for $n \geq 0$, define

$$B_n = (B - (n - 1) \cot \theta) \ldots (B - \cot \theta) B$$

and $B_{-n} = \overline{B_{-n}}$. From this we see that

$$X_{l,m}^n = \frac{1}{\sqrt{c_{nl}}^n} B_n Y_{l,m}^n.$$  

**Lemma 3.4.** With $B$ defined as in (20),

$$(B - n \cot \theta) \frac{1}{(\sin \theta)^k} Y_{l,m}^n = \frac{1}{(\sin \theta)^{k+1}} \frac{1}{2^l} [\frac{1}{(l-m+1)(l-n-k)} Y_{l+1,m} - \frac{1}{(l+m)(l+1+n+k)} Y_{l-1,m} - (2l+1)m Y_{l,m}]$$

and

$$(B + n \cot \theta) \frac{1}{(\sin \theta)^k} Y_{l,m}^n = \frac{1}{(\sin \theta)^{k+1}} \frac{1}{2^l} [\frac{1}{(l-m+1)(l+n-k)} Y_{l+1,m} - \frac{1}{(l+m)(l+1-n+k)} Y_{l-1,m} + (2l+1)m Y_{l,m}]$$

Consequently, we can now define the $X_{l,m}^n$ directly in terms of the scalar spherical harmonics.

**Corollary 3.5.** There are constants $c_{i,l,m}^n$ such that

$$X_{l,m}^n = \sum_{p=l-n}^{l+n} c_{i,l,m}^n \frac{1}{(\sin \theta)^{n+l}} Y_{p,m}$$

where the $c_{i,l,p,m}^n$ satisfy $c_{i,l,l,m}^0 = 1, c_{i,l,p,m}^0 = 0$ for $p \neq l$, $c_{i,l,p,-m}^n = c_{i,l,-p,m}^n$, and the recurrence relation

$$c_{i,l,p,m}^{n+1} = \frac{1}{\sqrt{l(l+1)-n(n+1)}} \left[ -m c_{i,l,p,m}^n + \frac{(p-m)(p-2n-1)}{2p-1} c_{i,l,p-1,m}^n + \frac{-(p+m+1)(p+2+2n)}{2p+3} c_{i,l,p+1,m}^n \right]$$

for $l-n \leq p \leq l+n, n \leq l$, and $c_{i,l,p,m}^n = 0$ for $p < l-n$ or $p > l+n$.

**Proof.** The first two properties of the $c_{i,p,m}^n$ are obvious. The third comes from the equation $X_{l,m}^n = X_{l,-m}^n$ which follows from the fact that $Y_{l,m} = Y_{l,-m}$, and hence $Y_{l,m} = Y_{l,-m}$. The recurrence relation comes from the identities of the previous lemma and the relation

$$X_{l,m}^{n+1} = \frac{1}{\sqrt{l(l+1)-n(n+1)}} (B - n \cot \theta) X_{l,m}^n.$$
Using Corollary 3.5 we can now give an algorithm for calculating the tensor spherical transform of type \( n \) for \(| n | \leq l \leq N \) using a single scalar spherical transform which we need only compute for all orders \( l \), with \( 0 \leq l \leq N + | n | \). Starting with a tensor field, \( \mathbf{f} \mathbf{e}_n \), we compute the auxiliary quantities

\[
g^n(l, m) = \left< \frac{1}{\sin \theta |m|} f \mathbf{Y}_m \right>
\]

for \( 0 \leq l \leq N + | n | \) using a scalar spherical transform. We then use the relations

\[
f^n(l, m) = \sum_{p=l-n}^{l+n} \xi_{l-p,m}^n g^n(p, m)
\]

to calculate the tensor harmonic transform in an additional \( (2n + 1) [(N + 1)^2 - n^2] \) scalar multiplications and \( 2n [(N + 1)^2 - n^2] \) scalar additions.

4. Sampling Theorems

In order to compute spherical harmonic transforms numerically, we must reduce them, at least approximately, to a finite problem. This means restricting ourselves to a finite number of Fourier coefficients, and representing functions by their values at a finite number of points. The simplest sampling theory is the band-limited theory, which explains how to reconstruct a polynomial on the sphere from its values at a finite number of points.

**Definition 4.1.** A tensor field \( \mathbf{f} \mathbf{e}_n \) of type \( n \), on \( S^2 \), is band-limited with band-limit \( B \), if \( f^n(l, m) = 0 \) for all \( l > B \). The space of such tensor fields is denoted \( F_B(E_n) \), so that

\[ F_B(E_n) = \text{span}_C \{ \mathbf{Y}_{lm}^n : |n|, |m| \leq l \leq B \}. \]

Let \( F(E_n) \) be the union of \( F_B(E_n) \) for all \( B > 0 \). In the case \( n = 0 \) we write \( F_B(E_0) = F_B = F(B(2)) \), and \( F = F(E_0) \).

The most important property of spaces of band-limited tensors is that the product of a tensor field of band-limit \( B_1 \), with a tensor field of band-limit \( B_2 \) has band-limit \( B_1 + B_2 \), i.e.,

**Lemma 4.1.** (i) \( F_{B_1}(E_{n_1}) \cap F_{B_2}(E_{n_2}) \subseteq F_{B_1 + B_2}(E_{n_1 + n_2}) \).

(ii) \( F_{B_1} \cdot F_{B_2}(E_n) \subseteq F_{B_1 + B_2} \).

Given a complex measure \( s \) on \( S^2 \), we define the **Fourier transform** of \( s \) to be the function

\[
\hat{s}(l, m) = \int_{S^2} Y_{lm} \overline{s} \, ds.
\]

If \( \mathbf{T} = \mathbf{f} \mathbf{e}_n \) is a continuous tensor field of type \( n \) on \( S^2 \), then we may form the product \( s \mathbf{T} \), and the spherical transform of this product is the function

\[
\tilde{s}(l, m) = \int_{S^2} \mathbf{X}_{lm} \overline{s} \, ds.
\]

When the tensor field is band-limited, there are simple conditions on the measure \( s \), to insure agreement of the low degree Fourier coefficients of \( \mathbf{T} \) and \( s \mathbf{T} \), defined as \{\( \hat{\mathbf{T}}(l, m) \)\} and \{\( \tilde{s}(l, m) \)\} respectively.

**Theorem 4.2** (Band-limited Sampling). Assume that \( s \) is a complex measure on \( S^2 \) such that \( \hat{s}(l, m) = \delta_{l,0} \) for \( |m| \leq l \leq 2B \), and \( \mathbf{T} \) is band-limited of band-limit \( B \). Then \( s \mathbf{T}(l, m) = \tilde{s}(l, m) \) for \( |m| \leq l \leq B \).
Figure 2. Plot of sample weights for range of problem sizes.

Proof. The condition on $s$ implies that as linear functionals, $s$ and the the invariant measure $\mu$ agree on the space $\mathcal{F}_{2B}$. Assume then, that this condition holds, and that $T$ is in $\mathcal{F}_{2B}(E_n)$ and $l \leq B$. Then $Y_{l,m}^{-n}$ is in $\mathcal{F}_{2B}(E_n)$, and by the lemma, $T \otimes Y_{l,m}^{-n}$ is in $\mathcal{F}_{2B}$. But $s(T(l,m)) = s(T \otimes Y_{l,m}^{-n})$.

The measure $s$ appearing in Theorem 4.2 shall be called the sampling measure.

The most commonly used sampling measures have support on either an equiangular grid or a Gaussian grid. For the algorithms discussed in the following sections, we shall use an equiangular grid, although a Gaussian grid (with points equally spaced in the $\varphi$ direction, and $\cos^{-1}(\theta)$ a root of a Legendre polynomial) is also possible. The following is a slight variation of the sampling theorem given in [19]. Sampling at the north pole and slightly different normalizing of the Legendre polynomials completely account for the differences between the expression for the weights $a_j$ and those given there ([19], p. 216).

Lemma 4.3. Let $s = \frac{B}{2B} \sum_{j=0}^{2B-1} \sum_{l=0}^{2B-1} a_j^{(l)} \delta(\theta_j, \varphi_k)$ where the sample points are chosen from the usual equiangular grid: $\theta_j = \pi(2j+1)/4B, \varphi_k = 2\pi k/2B$; and the weights $a_j$ have a closed form expression

\begin{equation}
    a_j = \frac{2}{B} \sin \left( \frac{\pi(2j+1)}{4B} \right) \sum_{k=0}^{B-1} \frac{1}{2k+1} \sin \left( \frac{(2j+1)(2k+1)}{4B} \right).
\end{equation}

Then $\hat{s}(l,m) = 0$ for $|m| \leq l \leq 2B - 1$.

In the case that the tensor field is not band-limited, Lemma 4.4 shows that via sampling we may still obtain an approximation to its Fourier coefficients.
Lemma 4.4. Assume $s$ is a measure on $S^2$ such that $\hat{s}(l,m) = \delta_{0,l}$ for $|m| \leq l \leq 2B$. Assume that $\mathbf{T}$ is a continuous tensor field of type $n$, and let $\mathbf{S} = s \cdot \mathbf{T}$. Then,

$$\sum_{l=|n|}^{B} (2l + 1) \left[ \sum_{|m| \leq l} \left( \hat{\mathbf{T}}(l,m) - \hat{s}(l,m) \right)^2 \right]^{\frac{1}{2}} \leq (B + 1)^2 (1 + 4B + B^2) ||s||_1 \sum_{B+1,|n| \leq l} (2l + 1) \left[ \sum_{|m| \leq l} \hat{\mathbf{T}}(l,m)^2 \right]^{\frac{1}{2}},$$

where $||s||_1$ is the total variation norm of $s$.

For a proof of this result see [44] or [43].

5. Computational harmonic analysis

Assume $s$ is a finitely supported measure on the sphere, $\mathbf{T}$ is a continuous tensor field of type $n$, and $B$ is a positive integer. We now consider the problem of computing the Fourier coefficients $\hat{s}(l,m)$ for $|n|, |m| \leq l \leq B$, given the values of $\mathbf{T}$ at the support of $s$. To see that this amounts to the computation of some finite sums, let $S$ be the support of $s$, and for each point $p$ in $S$, let $w_p$ be the weight associated with that point. $S$ is called the sampling set. Thus

$$s = \sum_{p \in S} w_p \delta_p.$$

Then, if $T = f \cdot e_n$, \(^1\) we have

$$s \cdot \mathbf{T}^n(l,m) = \sum_{p \in S} w_p f(p) \bar{\mathbf{T}}^n_{lm}.$$

The method we propose for this calculation reduces the problem to a number of simpler transforms.

The first reduction is to express the transforms for vector or tensor harmonics in term of scalar spherical harmonic transforms. We have already seen that the transform for a type $n$ tensor field may be written in terms of a single larger transform for complex functions.

The scalar spherical harmonic transform may be performed in two steps. First we calculate an intermediate transform using the functions $T_{lm} = T_l(\cos \theta)e^{-im\varphi}$ where $T_l$ is the degree $l$ Chebyshev polynomial. This may be done by well known algorithms for monomial or Chebyshev transforms. These algorithms work when the sampling set is a grid, but may also be adapted to many non-grid cases.

The second step in the spherical harmonic transform is to relate the transform for the $T_{lm}$ to the transform for the $Y_{lm}$. This is done using the techniques developed by Driscoll, Healy and Rockmore [19, 20].

\(^1\)If $S$ contains either the north or south pole, then we are forced to make a choice for the value of $e_n$ at the poles. The definition of $f$ at the poles will then reflect that choice, and $f$ will have a discontinuity there to match that of $e_n$. 

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5.1. Vector and Tensor Sphericals. Once we have a method of computing a spherical harmonic transform, the vector and tensor harmonic transforms are easy. For the vector case, equations (13)-(16) define how to express vector spherical coefficients in terms of scalar coefficients. For the tensor case, equations (21) and (22) are the critical ones.

The only thing which might give the reader pause is the computation of the “extra” scalar coefficients that are required to determine the highest degree vector and tensor coefficients. As is stated at the end of Section 3.1, the first step in calculating a tensor spherical transform of type \( n \) with band-limit \( B \) is to compute

\[
g^n(l, m) = \left\langle \frac{1}{(\sin \theta)^{1/2}} f, Y_{lm} \right\rangle
\]

for \( 0 \leq l \leq B + |n| \) using a scalar spherical transform. For nonzero \( n \), the computation of \( g^n(l, m) \) involves scalar spherical coefficients with degrees greater than the band-limit. Therefore we are projecting signals onto associated Legendre functions with degrees greater than the band-limit. The reason the final result makes sense is that the sampling theory needed to justify the computation only applies to the tensor fields \( f_{en} \). We do not need any sampling results to justify the validity of the scalar harmonic transforms in the intermediate stages of our computation.

6. Numerical Results

In this section we present results that indicate that a tensor spherical transform of type \( n \) can be performed in a stable fashion for a useful range of problem sizes (i.e., band-limits \( B \)) and ranks. For a detailed discussion of the stability and efficiency of several (non multipole-based) scalar spherical transform algorithms, we refer the reader to [32].

Experiments were performed on a DEC Alpha 500/200 and a SGI Origin 2000, and all code used was based on SpharmonicKit [58]. As noted in Section 2, the scalar spherical transform of a function \( f(\theta, \phi) \) is equivalent to a Fourier transform on the azimuthal angle \( \phi \) followed by an associated Legendre transform on the colatitude angle \( \theta \). To perform the scalar spherical transform, we used the “semi-naive” algorithm (as it is referred to in [32]). Originally developed by Dilts [18], this algorithm can compute the spherical transform of a function \( f \) in no more than \( O(B^3) \) operations. The Dilts algorithm takes advantage of the fact that the cosine expansion of an associated Legendre polynomial of degree \( l \) has at most \( l+1 \) non-zero terms. Although using this fact does not result in a discrete Legendre transform algorithm that is asymptotically faster than the naive algorithm, in practice it does allow for a faster (and still stable) algorithm. Also, although other algorithms are asymptotically faster than the semi-naive algorithm, we used the semi-naive algorithm in our experiments only as a matter of programming convenience. There is no reason to believe that using stable variations of other faster, but still stable, algorithms, would alter our results.

To measure the error of the tensor spherical algorithm, we employed the following procedure:

1. Select a band-limit \( B \) and rank \( n \).
2. Generate a set of random tensor spherical coefficients \( f_{lm}^n \), uniformly distributed between -1 and 1 for all legal values of \( l \) and \( m \), i.e., \( 0 \leq m \leq B, \max(m,n) \leq l \leq B \).
3. Synthesize the function

\[
\mathbf{v} = \sum_{|m|, |m| \leq l \leq B} \frac{1}{|Y_{lm}|^2} f_{lm}^n Y_{lm}^n
\]

4. Take the tensor spherical transform of the synthesized function, generating a new set of tensor spherical coefficients \( h_{lm}^n \).
5. Compute the error as

$$\max_{l,m} || f_{lm}^n - b_{lm}^n ||.$$ 

6. Repeat steps 2-5 ten times.

7. Compute the average absolute and relative errors over the ten trials.

Comments concerning the synthesis done in Step 3 will be made at the end of this section. Also, the random coefficients were chosen so that the resulting function samples would be strictly real. Furthermore, the “extra” Legendre coefficients were calculated using the naive Legendre transform.

Originally we represented floating point numbers using the 8-byte long C data type double. However, we later discovered that on the Origin (and not the DEC) we could gain noticeable (though not dramatically greater) accuracy by using the 16-byte long data type long double. On our DEC, doubles and long doubles are both 8-bytes long.

In Table 1 we give the absolute and relative errors for tensor spherical transforms of different ranks at different band-limits. As can be seen, the error grows worse as the band-limit and rank increase. The source of this poor behavior can easily be identified. Recall that in order to calculate the tensor spherical coefficients, we first compute

$$g^n(l, m) = \left\langle \frac{1}{(\sin \theta)^{|m|}} f, Y_{lm} \right\rangle_{\text{disc}}$$

where $n$ is the rank of the transform. The subscript “disc” is to remind us that we are now dealing with the discrete inner product. To calculate $g^n(l, m)$, we first divide the sampled signal $f$ by $(\sin \theta)^{|m|}$ and then take the scalar transform of that modified signal.

In Figure 3 we have plotted $1/(\sin \theta)^{|m|}$ for different ranks $n$ at band-limit $= 255$. Dividing the sampled function $f$ by $(\sin \theta)^{|m|}$ is “blowing up” those sample values near the ends of the interval. Consequently, accuracy deteriorates as the rank increases. And as the band-limit gets larger, this deterioration simply becomes worse at an even faster rate.

Although the source of the instability cannot be entirely removed, we can easily lessen its influence, at least to some extent. To do so, we must consider the weights used in the Legendre-transform portion of the scalar spherical transform.
Figure 3. $1/(\sin \theta_j)^{n_1}$ for ranks $n = 1, 2$ and $3$ at bandwidth 255.

By Lemma 4.3, we see that the weights can be written as a product of $\sin \theta$ and a sum involving sines. Therefore, we can “move” one of the sines in $(\sin \theta)^{n_1}$ over to the expression for the weights, and hence remove one occurrence of dividing by $\sin \theta$. That is, eqn. (24) now becomes

$$g^n(l, m) = \left< \frac{1}{(\sin \theta)^{n_1}} f, Y_m \right>_{\text{disc}}$$

(25)

$$= \left< \frac{1}{(\sin \theta)^{n_1-1}} f, Y_m \right>_{\text{disc-1}}$$

The subscript “disc-1” in the above equation means that this discrete inner product is computed using sampling weights $a_j$ (eqn. (23)) which have been divided by $\sin \theta$.

In practice we have found that it is possible to move $\sin^2 \theta$ over to the weights and gain noticeable improvement of accuracy, but that moving larger powers of $\sin \theta$ to the weights does not seem so useful. Hence, the inner product we are evaluating is

$$g^n(l, m) = \left< \frac{1}{(\sin \theta)^{n_1}} f, Y_m \right>_{\text{disc}}$$

(26)

$$= \left< \frac{1}{(\sin \theta)^{n_1-2}} f, Y_m \right>_{\text{disc-2}}$$

In Figure 4 we plot the original and modified weights for bandwidth = 255. Using weights modified by moving $\sin^2 \theta$ (i.e., the weights plotted in the bottom of Figure 4), we obtained the absolute and relative errors given in Table 2. In order to obtain as much accuracy as possible, all modified weights used were computed in Mathematica® and then saved to disk. The C code reads in the weights as needed.
In another attempt to gain additional accuracy, we used the C language data type long double on the SGI, which is 16 bytes long. (Recall that long double on our DEC Alpha is only 8 bytes long.) The error results obtained using this data type are given in Table 3. Comparing Tables 2 and 3, we see that the ability to use a 16-byte long double does improve accuracy somewhat. In the event that a given platform does not provide the “long” long double datatype, we see no reason why a software means of getting around this hardware limitation cannot be used. For example, it should be possible to use the GMP (GNU Multi-Precision) library in order to gain further precision, albeit at the cost of increased execution time. However, we admit that we have not tried this and there may be difficulties in such an implementation.
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Table 3. Tensor spherical transforms: absolute (first row) and relative (second row) errors for different band-limits and ranks using the modified (by $\sin^2 \theta$) weights. Floating point numbers represented using the C language type long double on the SGI.

6.1. The Errors: A Closer Look. In Table 3 we give the absolute and relative errors of the tensor transform algorithm for different band-limits and ranks using the modified weights. Consider the errors at band-limit = 255. For ranks $n = 1, 2, 3$, the errors seem acceptable (at least to us!), for $n = 4$, less so. In order to examine the behavior of the errors more closely, we took the error results of one iteration of the test loop and plotted the maximum absolute and relative errors at each order $m$. That is, given the coefficients computed at order $m$, calculate the largest absolute and relative error of these coefficients, and do this for all orders $0 \leq m \leq 255$. In Figures 5 and 6 we show semilog plots of the errors for orders $m = 0, \ldots, 50$, for different rank transforms. Note how the errors quickly decay as the order increases. As is obvious in the plots, the largest errors occur at those values of the order $m$ for which $m$ is near the rank $n$ of the transform. The cause of this phenomenon can be identified using the relation between associated Legendre functions and Gegenbauer polynomials.

Associated Legendre functions may be expressed in terms of Gegenbauer polynomials:

$$P_{lm}(\cos \theta) = A_{lm} \sin^m \theta \times C_{l-m,m+1/2}(\cos \theta)$$

where $A_{lm}$ is a normalizing constant and $C_{l-m,m+1/2}(\cos \theta)$ denotes a Gegenbauer polynomial. Note the presence of the $\sin^m \theta$. When the order $m$ is greater than the rank $n$ of the transform, we are effectively no longer dividing by a power of $\sin \theta$. In other words, the higher order associated Legendre functions “absorb” all occurrences of $\sin \theta$. So nowhere is division by small $\sin \theta$ taking place.

Therefore, we conjecture that it is possible to do a still reasonably fast tensor spherical transform, for a reasonable rank at a reasonable band-limit. Extra precision is required only for computing the low order coefficients. The majority of coefficients, for orders $m$ greater than the rank $n$ could still be computed without special extended (i.e., slow) precision “handling”.

6.2. The Synthesis. In Step 3 of our procedure for measuring the error of a rank $n$ tensor spherical algorithm, we synthesize the function

$$v = \sum_{|\ell_1|,|\ell_2| \leq B} \frac{1}{|Y_{lm}|^2} f^n_{lm} Y^n_{lm}$$
where $f_{im}^n$ were randomly generated tensor spherical coefficients. By the definition of $Y_{im}^n$ (Corollary 3.5), this involves dividing a sampled scalar spherical harmonic $Y_{im}$ by $(\sin \theta)^{|n|}$. From the results we have presented, we know that the principle source of error in evaluating the inner products is the division by $(\sin \theta)^{|n|}$. By moving $\sin^2 \theta$ over to the weights, the error is somewhat (though not greatly) reduced.
However, since division by $(\sin \theta)^{|m|}$ is part of the synthesis step, a legitimate question to ask is how much error is present in the sampled function $v$ itself, before any spherical transforms are computed. Reporting error values obtained from the use of dubious sampling data would not be of much value. We want to test the tensor algorithm and not the sampling+tensor algorithm. To accomplish this, we used Mathematica®.
As a means of testing the tensor algorithm alone, we ran the following experiment. For band-limit $B = 255$ and rank $n = 4$, we set the tensor coefficients as follows:

\[ f_{lm}^n = \begin{cases} 
1 & \text{if } m \geq 0, \\
0 & \text{else.} 
\end{cases} \]

Next, we sampled $v$ in Mathematica®. This sampling can be done at high precision and we can control this precision too. The sample values generated were then written to disk and it was this data that was read into the C code and tensor-transformed. The differences between the errors obtained using the Mathematica® data as input data and the errors produced using the C-generated input data were minimal. Therefore, the errors we are seeing are not entirely due to the sampling. Those errors really do result when the tensor transform algorithm is implemented in a finite-precision fashion.

7. Conclusion

We have described algorithms for the numerical computation of Fourier transforms of tensor fields on the two-sphere, $S^2$. These algorithms reduce the computation of an expansion on tensor spherical harmonics to expansions in scalar spherical harmonics, and hence can take advantage of improvements in the computation of scalar spherical harmonic transforms.

Although the algorithms we describe are susceptible to certain numerical instabilities, we present numerical results which indicate that minor variations of the algorithms can produce stable results for a useful range of band-widths and ranks.

References


[28] SphericalKit is a freely available collection of C programs for doing Legendre and scalar spherical transforms. Developed at Dartmouth College by S. Moore, D. Healy, D. Rockmore and P. Kostelec, it is available at www.cs.dartmouth.edu/~spherical/sphere.


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