Fast and backward stable transforms between spherical harmonic expansions and bivariate Fourier series



Richard Mikael Slevinsky

Department of Mathematics, University of Manitoba

Richard.Slevinsky@umanitoba.ca

OPSFA

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Spherical Harmonics



Let μ be a positive Borel measure on $D \subset \mathbb{R}^n$. The inner product:

$$\langle f,g\rangle = \int_D \overline{f(x)}g(x) \,\mathrm{d}\mu(x),$$

induces the norm $\|f\|_2 = \sqrt{\langle f, f \rangle}$ and the Hilbert space $L^2(D, d\mu(x))$.

Let $\mathbb{S}^2 \subset \mathbb{R}^3$ denote the unit 2-sphere and let $d\Omega = \sin \theta \, d\theta \, d\varphi$. Then any function $f \in L^2(\mathbb{S}^2, \, d\Omega)$ may be expanded in spherical harmonics:

$$f(\theta,\varphi) \sim \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{+\ell} f_{\ell}^{m} Y_{\ell}^{m}(\theta,\varphi) = \sum_{m=-\infty}^{+\infty} \sum_{\ell=|m|}^{+\infty} f_{\ell}^{m} Y_{\ell}^{m}(\theta,\varphi),$$

where the expansion coefficients are:

$$f_{\ell}^{m} = \int_{\mathbb{S}^{2}} \overline{Y_{\ell}^{m}(\theta, \varphi)} f(\theta, \varphi) \,\mathrm{d}\Omega.$$

Spherical Harmonics



Spherical harmonics are defined by:

$$Y_{\ell}^{m}(\theta,\varphi) = \frac{e^{\mathrm{i}m\varphi}}{\sqrt{2\pi}} \underbrace{\mathrm{i}^{m+|m|} \sqrt{(\ell+\frac{1}{2}) \frac{(\ell-m)!}{(\ell+m)!}} P_{\ell}^{m}(\cos\theta)}, \quad \ell \in \mathbb{N}_{0}, \quad -\ell \leq m \leq \ell.$$

Associated Legendre functions are defined by ultraspherical polynomials:

$$P_{\ell}^{m}(\cos\theta) = (-2)^{m}(\frac{1}{2})_{m}\sin^{m}\theta C_{\ell-m}^{(m+\frac{1}{2})}(\cos\theta).$$

The notation \tilde{P}_{ℓ}^m is used to denote orthonormality, and:

$$(x)_n = \frac{\Gamma(x+n)}{\Gamma(x)}$$

is the Pochhammer symbol for the rising factorial.

Spherical Harmonics



Consider the Laplace–Beltrami operator on \mathbb{S}^2 :

$$\Delta_{\theta,\varphi} = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2}.$$

For $\ell \in \mathbb{N}_0$ and $|m| \leq \ell$, the surface spherical harmonics are the eigenfunctions of $\Delta_{\theta,\varphi}$:

$$\Delta_{\theta,\varphi} Y_{\ell}^{m}(\theta,\varphi) = -\ell(\ell+1)Y_{\ell}^{m}(\theta,\varphi).$$

Spherical harmonics diagonalize the Laplace-Beltrami operator.

Real-(World) Applications





- Global Numerical Weather Prediction (NWP). Global climate models at the *European Centre for Medium-Range Weather Forecasts* use spherical harmonics to represent the world's climate with a horizontal resolution of approximately 10 km, corresponding to roughly 64 million degrees of freedom.
- Analysis of the Planck experiment. The *European Space Agency* sent the *PLANCK* satellite in orbit in 2013 to collect cosmic background radiation in an attempt to observe the first light of the universe. High resolution data are analyzed by spherical harmonics.
- Time-dependent Schrödinger equation in angular coordinates:

$$\mathrm{i}\hbarrac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)
angle=\left(\hat{\mathcal{T}}+\hat{\mathcal{V}}(t)
ight)|\Psi(t)
angle,\qquad|\Psi(t_0)
angle=|\Psi_0
angle,$$

models polarization effects.

Time Evolution



• Many real-world applications may be abstracted to semi-linear PDEs:

$$u_t = \mathcal{L}u + \mathcal{N}(u, t), \qquad u(t_0) = u_0.$$

where ${\cal L}$ is a linear (differential) operator, and ${\cal N}$ is not.

- Usually, $\mathcal{L} = \Delta$ or something similar and $\mathcal{N}(u, t) = u^2$, for example.
- Higher-order derivatives in time are reformulated as a system.
- Many algorithms exist for semi-linear time-stepping:
 - Operator splitting preserves unitarity;
 - Exponential integrating integrates the stiff linear term exactly; and,
 - Implicit-explicit schemes are designed for versatility & efficiency.
- Problem: \mathcal{L} is localized in momentum (coefficient) space and \mathcal{N} is localized in physical (value) space.

Problem



Fast transforms are required to convert between representations in momentum and physical spaces:

Synthesis Convert an expansion in spherical harmonics to function values on the sphere.

Analysis Convert function values on the sphere to spherical harmonic expansion coefficients.

For a band-limit of $\ell \leq n$, the naïve cost is $\mathcal{O}(n^4)$ but it can be trivially reorganized to $\mathcal{O}(n^3)$. The goal is a run-time of $\mathcal{O}(n^2 \log^{\mathcal{O}(1)} n)$. This has a rich history, including works by Driscoll and Healy, Mohlenhamp, Suda and Takami, Kunis and Potts, Rokhlin and Tygert and Tygert. Questions about current approaches:

- Which grids should be chosen? If tensor-product grids, should they be Gaussian or equispaced-in-angle?
- Is the method numerically stable? Important for time evolution.



The sphere is doubly periodic and supports a bivariate Fourier series.

- The FFT, DCT, and DST solve synthesis and analysis.
- Nonuniform variants extend this to arbitrary grids.
- $Y_{\ell}^{m}(\theta,\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}} \tilde{P}_{\ell}^{m}(\cos\theta) \Rightarrow \text{ in longitude, we are done.}$
- The problem is to convert $\tilde{P}_{\ell}^m(\cos\theta)$ to Fourier series.
- Since $\tilde{P}_{\ell}^{m}(\cos\theta) \propto \sin^{m}\theta C_{\ell-m}^{(m+\frac{1}{2})}(\cos\theta)$,
 - even-ordered \tilde{P}_{ℓ}^{m} are trigonometric polynomials in $\cos \theta$; and,
 - odd-ordered \tilde{P}_{ℓ}^m are trigonometric polynomials in $\sin\theta.$
- Conversions are *not* one-to-one.

The SH Connection Problem



Definition

- Let $\{\phi_n(x)\}_{n\geq 0}$ be a family of orthogonal functions with respect to $L^2(\tilde{D}, d\tilde{\mu}(x))$; and,
- let $\{\psi_n(x)\}_{n\geq 0}$ be another family of orthogonal functions with respect to $L^2(D, d\mu(x))$.

The connection coefficients:

$$c_{\ell,n} = \frac{\langle \psi_{\ell}, \phi_n \rangle_{\mathrm{d}\mu}}{\langle \psi_{\ell}, \psi_{\ell} \rangle_{\mathrm{d}\mu}},$$

allow for the expansion:

$$\phi_n(x) \sim \sum_{\ell=0}^{\infty} c_{\ell,n} \psi_\ell(x).$$



Theorem

Let $\{\phi_n(x)\}_{n\geq 0}$ and $\{\psi_n(x)\}_{n\geq 0}$ be two families of orthonormal functions with respect to $L^2(D, d\mu(x))$. Then the connection coefficients satisfy:

$$\sum_{\ell=0}^{\infty} \overline{c_{\ell,m}} c_{\ell,n} = \delta_{m,n}.$$

- Any matrix $A \in \mathbb{R}^{m \times n}$, $m \ge n$, with orthonormal columns is well-conditioned and Moore–Penrose pseudo-invertible $A^+ = A^\top$.
- For every *m*, the P^m_ℓ(x) are a family of orthonormal functions for the same Hilbert space L²([-1, 1], dx).

The SH Connection Problem



Definition

Let G_n denote the Givens rotation:

$$G_n = \begin{bmatrix} 1 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & c_n & 0 & s_n & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -s_n & 0 & c_n & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{bmatrix},$$

where the sines and the cosines are in the intersections of the n^{th} and $n + 2^{nd}$ rows and columns, embedded in the identity of a conformable size.

The SH Connection Problem



Theorem

The connection coefficients between $\tilde{P}_{n+m+2}^{m+2}(\cos\theta)$ and $\tilde{P}_{\ell+m}^{m}(\cos\theta)$ are:

$$c_{\ell,n}^{m} = \begin{cases} (2\ell + 2m + 1)(2m + 2)\sqrt{\frac{(\ell + 2m)!}{(\ell + m + \frac{1}{2})\ell!}\frac{(n + m + \frac{5}{2})n!}{(n + 2m + 4)!}}, & \text{for} \quad \ell \le n, \quad \ell + n \text{ even}, \\ -\sqrt{\frac{(n + 1)(n + 2)}{(n + 2m + 3)(n + 2m + 4)}}, & \text{for} \quad \ell = n + 2, \\ 0, & \text{otherwise}. \end{cases}$$

Furthermore, the matrix of connection coefficients $C^{(m)} = G_0^{(m)} G_1^{(m)} \cdots G_{n-2}^{(m)} G_{n-1}^{(m)} I_{(n+2) \times n}$, where the sines and cosines are:

$$s_n^m = \sqrt{rac{(n+1)(n+2)}{(n+2m+3)(n+2m+4)}}, \quad ext{and} \quad c_n^m = \sqrt{rac{(2m+2)(2n+2m+5)}{(n+2m+3)(n+2m+4)}}.$$



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"Proof." W.l.o.g., consider m = 0 and n = 6.

	(0.91287	0.0	0.31623	0.0	0.17593	0.0
	0.0	0.83666	0.0	0.39641	0.0	0.24398
	-0.40825	0.0	0.70711	0.0	0.3934	0.0
$C^{(0)}$	0.0	-0.54772	0.0	0.60553	0.0	0.37268
	0.0	0.0	-0.63246	0.0	0.5278	0.0
	0.0	0.0	0.0	-0.69007	0.0	0.46718
	0.0	0.0	0.0	0.0	-0.73193	0.0
	0.0	0.0	0.0	0.0	0.0	-0.76376

The SH Connection Problem



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"Proof." Apply the Givens rotation $G_0^{(0)\top}$:

	(1.0	0.0	0.0	0.0	0.0	0.0 \
	0.0	0.83666	0.0	0.39641	0.0	0.24398
	0.0	0.0	0.7746	0.0	0.43095	0.0
$C^{(0)\top}C^{(0)}$	0.0	-0.54772	0.0	0.60553	0.0	0.37268
$G_0 + C =$	0.0	0.0	-0.63246	0.0	0.5278	0.0
	0.0	0.0	0.0	-0.69007	0.0	0.46718
	0.0	0.0	0.0	0.0	-0.73193	0.0
	0.0	0.0	0.0	0.0	0.0	-0.76376/

The SH Connection Problem



	(1.0	0.0	0.0	0.0	0.0	0.0
	0.0	1.0	0.0	0.0	0.0	0.0
	0.0	0.0	0.7746	0.0	0.43095	0.0
$C^{(0)\top}C^{(0)\top}C^{(0)}$	0.0	0.0	0.0	0.72375	0.0	0.44544
$G_1 G_0 C =$	0.0	0.0	-0.63246	0.0	0.5278	0.0
	0.0	0.0	0.0	-0.69007	0.0	0.46718
	0.0	0.0	0.0	0.0	-0.73193	0.0
	\0.0	0.0	0.0	0.0	0.0	-0.76376/



$$G_2^{(0)\top} G_1^{(0)\top} G_0^{(0)\top} C^{(0)} = \begin{pmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.72375 & 0.0 & 0.44544 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.68139 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & -0.69007 & 0.0 & 0.46718 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -0.73193 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -0.76376 \end{pmatrix}$$



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	/1.0	0.0	0.0	0.0	0.0	0.0
	0.0	1.0	0.0	0.0	0.0	0.0
	0.0	0.0	1.0	0.0	0.0	0.0
0)	0.0	0.0	0.0	1.0	0.0	0.0
' =	0.0	0.0	0.0	0.0	0.68139	0.0
	0.0	0.0	0.0	0.0	0.0	0.6455
	0.0	0.0	0.0	0.0	-0.73193	0.0
	0.0	0.0	0.0	0.0	0.0	-0.76376/

$$G_3^{(0)\top} G_2^{(0)\top} G_1^{(0)\top} G_0^{(0)\top} C^{(0)} =$$



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$$G_{4}^{(0)\top}G_{3}^{(0)\top}G_{2}^{(0)\top}G_{1}^{(0)\top}G_{0}^{(0)\top}C^{(0)} = \begin{pmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.6455 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ \end{pmatrix}$$

The SH Connection Problem



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"Proof." And finally:

$$G_{5}^{(0)\top} G_{4}^{(0)\top} G_{3}^{(0)\top} G_{2}^{(0)\top} G_{1}^{(0)\top} G_{0}^{(0)\top} C^{(0)} = \begin{bmatrix} 0.0 & 1.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \\ 0.0 & 0.0 \end{bmatrix}$$

(1.0	0.0	0.0	0.0	0.0	0.0
0.0	1.0	0.0	0.0	0.0	0.0
0.0	0.0	1.0	0.0	0.0	0.0
0.0	0.0	0.0	1.0	0.0	0.0
0.0	0.0	0.0	0.0	1.0	0.0
0.0	0.0	0.0	0.0	0.0	1.0
0.0	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0/

The SH Connection Problem



"Proof." Schematically:



• Conversion between neighbouring layers is $\mathcal{O}(n)$ flops and storage.

• The Givens rotations are computed to high relative accuracy due to analytical expressions of sines and cosines ⇒ **backward stable**.



Spherical Harmonics to Fourier



- Convert high-order layers to layers of order 0 and 1 in $\mathcal{O}(n^3)$ flops and $\mathcal{O}(n^2)$ storage; and,
- Convert low-order layers to Fourier series in O(n² log n) flops and O(n log n) storage à la Fast Multipole Method.

To make an algorithm fast, we usually need to make approximations.

A Fast Transform



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To convert high-order layers to layers of order 0 and 1 in $\mathcal{O}(n^2 \log^2 n)$ flops, we need something more.

For $m \in \mathbb{N}$, the connection coefficients between $\tilde{P}^{2m}_{\ell+2m}$ and \tilde{P}^0_n are given by the inner product:

$$c_{\ell,n}^{2m} = \int_{-1}^{1} \tilde{P}_{\ell+2m}^{2m}(x) \tilde{P}_n^0(x) \,\mathrm{d}x.$$

Using the Fourier transform of \tilde{P}_n^0 :

$$c_{\ell,n}^{2m} = \frac{(-\mathrm{i})^n \sqrt{n+\frac{1}{2}}}{\pi} \int_{\mathbb{R}} j_n(k) \,\mathrm{d}k \int_{-1}^1 e^{\mathrm{i}kx} \tilde{P}_{\ell+2m}^{2m}(x) \,\mathrm{d}x.$$

The matrix of connection coefficients is an operator composition with the variables $(n \times k) \times (k \times x) \times (x \times \ell)$. The Fourier integral operator is special.



- **Purpose:** Abstract the algebra of the FFT.
- **Technique:** Divide-and-conquer \Leftrightarrow merge-and-split.
- Technology: The interpolative decomposition.
 - **Proof:** Fourier integral operators have *rank-proportional-to-area*.
- The ranks of operator compositions are bounded by the smallest rank in the composition, extending applicability beyond Fourier integral operators.

The Interpolative Decomposition

Lemma

Let $A \in \mathbb{R}^{m \times n}$. For any k, there exist $A_{CS} \in \mathbb{R}^{m \times k}$ whose columns are a unique subset of the columns of A and $A_{I} \in \mathbb{R}^{k \times n}$ such that:

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- Some subset of the columns of A_I makes up the k × k identity matrix;
 ∥vec(A_I)∥_∞ ≤ 1;
- the spectral norm of $A_{\rm I}$ satisfies $\|A_{\rm I}\|_2 \leq \sqrt{k(n-k)+1}$;
- Ithe least singular value of A_I is at least 1;

•
$$A_{CS}A_{I} = A$$
 whenever $k = m$ or $k = n$; and,

• when $k < \min\{m, n\}$, the spectral norm of $A - A_{CS}A_{I}$ satisfies:

$$\left\|A - A_{\rm CS}A_{\rm I}\right\|_2 \leq \sqrt{k(n-k) + 1}\sigma_{k+1}.$$

where σ_{k+1} is the $k + 1^{st}$ singular value of A.

We say that $A \approx A_{\rm CS}A_{\rm I}$ and any structure in A is also in $A_{\rm CS}$.



Step 1: Partition $A \in \mathbb{R}^{n \times n}$ into thin strips. Compute IDs of each subblock.





Step 2 (a): Merge the strips and split them approximately in half.





Step 2 (b): Compute IDs of each subblock.





Step 3 (a): Again, merge the strips and split them approximately in half.





Step 3 (b): Compute IDs of each subblock.



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Step 4 (a): Final step, merge the strips and split them approximately in half.





Step 4 (b): Final step, compute IDs of each subblock.





Let $A \in \mathbb{R}^{n \times n}$ have rank-proportional-to-area.

- Every time we merge-and-split, the complexity of a matrix-vector product is approximately halved.
- We have created a permuted and sparse block-diagonal factorization.
- Costs $\mathcal{O}(k_{\text{avg}}n^2)$ to compute the factorization and $\mathcal{O}(k_{\text{avg}}n \log n)$ for a matrix-vector product, where k_{avg} is the average rank of all IDs.

To convert all associated Legendre functions to orders 0 and 1, requires $\mathcal{O}(k_{\text{avg}}n^3)$ flops to pre-compute and $\mathcal{O}(k_{\text{avg}}n^2 \log n)$ to apply.



Spherical Harmonics to Fourier



- Convert high-order layers to layers of order 0 and 1 in O(k_{avg} n² log n) flops and O(k_{avg} n² log n) storage; and,
- Convert low-order layers to Fourier series in O(n² log n) flops and O(n log n) storage à la Fast Multipole Method.

Chebyshev–Legendre Transform



Definition

The meromorphic function $\Lambda : \mathbb{C} \to \mathbb{C}$ is defined by:

$$\Lambda(z) := rac{\Gamma(z+rac{1}{2})}{\Gamma(z+1)}$$

For z sufficiently large,

$$\Lambda(z) pprox \left(1 - rac{1}{64(z+rac{1}{4})^2} + rac{21}{8,192(z+rac{1}{4})^4} + \dots +
ight) \left/ \sqrt{z+rac{1}{4}}
ight.$$

and otherwise:

$$\frac{\Lambda(z+1)}{\Lambda(z)} = \frac{z+\frac{1}{2}}{z+1}.$$

Chebyshev–Legendre Transform



Conversion from \tilde{P}_n^0 to cosines is given by:

$$\tilde{P}_n^0(\cos\theta) = \sqrt{n+\frac{1}{2}} \sum_{\ell=n,-2}^0 \Lambda(\frac{n-\ell}{2}) \Lambda(\frac{n+\ell}{2}) \frac{2-\delta_{\ell,0}}{\pi} \cos\ell\theta.$$

Inversely:

$$\cos n\theta = -n \sum_{\ell=n,-2}^{0} \frac{\Lambda(\frac{n-\ell-2}{2})\Lambda(\frac{n+\ell-1}{2})}{(n-\ell)(n+\ell+1)} \sqrt{\ell+\frac{1}{2}} \tilde{P}_{\ell}^{0}(\cos \theta).$$

Similar expressions exist for converting \tilde{P}_n^1 to sines.



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Many methods convert between Chebyshev and Legendre expansions:

- Using asymptotics, Legendre polynomial oscillations are localized in frequency;
- Using a fast partial Cholesky decomposition, the diagonally-scaled Toeplitz-dot-Hankel structure may be exploited; or,
- Using an adaptation of the **Fast Multipole Method**, subblocks of connection coefficients well-separated from the main diagonal are well-approximated by low-rank matrices.

Fast Multipole Method



The method, due to Greengard and Rokhlin, originates from the *multipole expansion* of the Coulombic potential:

$$\frac{1}{|\mathbf{r} - \mathbf{r}_0|} = \frac{1}{\sqrt{r^2 - 2rr_0\cos\theta + r_0^2}} = \frac{1}{r}\sum_{n=0}^{\infty} \left(\frac{r_0}{r}\right)^n P_n(\cos\theta).$$

Expansion for sufficiently small $r_0/r \ll 1$,

 $\Leftrightarrow \mathcal{O}(\log(\varepsilon^{-1})) \text{ terms in the multipole expansion for approximation to precision } \varepsilon,$

 \Leftrightarrow Subblocks well-separated from the main diagonal.

Alpert and Rokhlin use FMM to accelerate the Chebyshev–Legendre transform.

What does well-separation resemble?

Fast Multipole Method



An upper-triangular matrix with subblocks well-separated from the main diagonal:





Spherical Harmonics to Fourier



- Convert high-order layers to layers of order 0 and 1 in $\mathcal{O}(k_{\text{avg}}n^2 \log n)$ flops and $\mathcal{O}(k_{\text{avg}}n^2 \log n)$ storage; and,
- Convert low-order layers to Fourier series in $\mathcal{O}(n^2 \log n)$ flops and $\mathcal{O}(n \log n)$ storage à la Fast Multipole Method.

Can we beat $\mathcal{O}(k_{\text{avg}}n^3)$ pre-computation?

Skeletonizing the Pre-Computation 😓



No, but skeletonizing the pre-computation makes it practical for a laptop. Neighbouring layers are converted via Given rotations.





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Numerical Results: Slow





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Numerical Results: Slow





Numerical Results: Fast





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Numerical Results: Fast





Numerical Results: Fast





Numerical Results: Fast



Conclusion & Outlook



- New transforms are created to convert spherical harmonic expansions into bivariate Fourier series.
- They are asymptotically fast, O(n² log² n), and backward stable by construction. For practical band-limits of n ≤ O(10,000), the asymptotically optimal complexity does not yet appear.
- They are freely available in JULIA in FastTransforms.jl.
- A straightforward extension to conversion of Zernike polynomials to Fourier–Chebyshev series on the unit disk.
- A similar approach might extend to more exotic bivariate orthogonal polynomials on triangles.
- Is there a pre-computation-free method?

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