Fast Transforms and a Nonlocal Vector Calculus on the Sphere

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1 Koornwinder Polynomials

Koornwinder describes a constructive procedure to generate bivariate analogues of Jacobi polynomials. E.g.
- spherical harmonics $Y_\ell^m(\theta,\varphi)=(\sin\theta)^{|m} \mid \tilde{P}_{\ell-|m|}^{(|m|,|m|)}(\cos\theta)\frac{e^{im\varphi}}{\sqrt{2\pi}}$;
- Zernike polynomials $Z_l^m(r,\theta)=\sqrt{2\ell+2}r^m P_{\frac{i-m}{2}}^{(0,lm)}\left(2r^2-1\right)\frac{e^{im\theta}}{\sqrt{2\pi}}$;
- Proriol polynomials

$$\tilde{P}_{f,m}^{(\alpha,B,\gamma)}(x,y)=(2-2x)^m\tilde{P}_{f-m}^{(2m+\beta+\gamma+1,\alpha)}(2x-1)\tilde{P}_m^{(\gamma,\beta)}\left(\frac{2y}{1-x}-1\right)$$

orthogonal on the triangle. They have different applications but they share many properties: they are separable in some coordinate system; but in the ambient coordinates, there may be singularities such as $(\sin\theta)^{|m|}$ for spherical, $r^{|m|}$ for Zernike, and $(2-2x)^m$ for Proriol.

2 Spherical Harmonics

μ be a positive Borel measure on D.

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

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 $\mathrm{d}\Omega=\sin\theta\mathrm{d}\theta\mathrm{d}$ Then any function $f\in L^2\left(\mathbb{S}^2,\ \mathrm{d}\Omega\right)$ may be expanded in spherical harmonics:

$$f(\theta,\varphi)=\sum_{l=0}^{+\infty}\sum_{m=-l}^{+l}f_l^mY_l^m(\theta,\varphi)=\sum_{m=-\infty}^{+\infty}\sum_{l=|m|}^{+\infty}f_l^mY_l^m(\theta,\varphi)$$

where the expansion coefficients are:

$$f_l^m = \frac{\langle Y_l^m, f\rangle}{\langle Y_l^m, Y_l^m\rangle}$$

For $l \in \mathbb{N}_0$ and $|m| \leq l$, orthonormal spherical harmanics. Associated Legendre functions are defined by ultraspherical polynomials:

$$P_l^m(\cos\theta) = (-2)^m \left(\frac{1}{2}\right)_m \sin^m \theta C_{l-m}^{(m+\frac{1}{2})}(\cos\theta)$$

The notation $\tilde{P}_r^m$ is used to denote orthonormality, and

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

is the Pochhammer symbol for the rising factorial.

3 Applications

Global weather numerical predictions (climate models), analysis of planck experiment, time evolution of nonlocal reaction-diffusion equations, etc.
Semi-linear PDEs with nonlocal diffusion have many applications:

$$u_t = \epsilon^2 \mathcal{L}_\delta u + \mathcal{N}(u), \quad u(t=0,x) = u_0(x). \quad \epsilon > 0$$

where $\mathcal{L}_\delta$ is a linear nonlocal operator, and $\mathcal{N}$ is not Our nonlocal model is:

$$\mathcal{L}_\delta u(\mathbf{x}) = \int_{\mathfrak{d}^2} \rho_\delta(|\mathbf{x}-\mathbf{y}|)[u(\mathbf{y}) - u(\mathbf{x})]d\Omega(\boldsymbol{y})$$

The kernel ρ_δ is nonnegative and compactly supported by a horizon $0 < \delta \leq 2$ For example, $\mathcal{N}(u) = u - u^3$ in the Allen-Cahn equation.
Problem: r is localized in momentum (coefficient) space and $\mathcal{N}$ is localized in physical (value) space.

4 Synthesis and Analysis

A band-limited function of degree n on the sphere has no nonzero spherical harmonic expansion coefficient of degree n or greater.

$$f_{n-1}(\theta.\varphi) = \sum_{t=0}^{n-1} \sum_{m=-l}^{+l} f_l^m Y_l^m(\theta.\varphi)$$

For a spherical harmonic Y_l^m, l is the degree and m is the order. The transforms of synthesis and analysis convert between representations of a band-limited function in momentum and physical spaces: Synthesis Sample a band-limited function at a set of points on $\mathbb{S}^2$. Analysis Convert samples on $\mathbb{S}^2$ to spherical harmonic expansion coefficients.

Normally an appropriate set of points is chosen to be able to perfectly reconstruct a band-limited function of degree n. Point sets include:
Equiangular θ_k and φ_j are equispaced and their Cartesian product is taken. These include the celebrated Driscoll-Healy (2 n)(2 n-1) and McEwen-Wiaux (n-1)(2 n-1)+1 sampling theorems.
Gaussian $\cos\theta_k$ are Gauss-Legendre points and their Cartesian product is taken.
HEALPix procedure to generate points that correspond to a hierarchical equal area isolatitude pixelization of S^2.
Random with common distributions.
Data-driven may be treated similar to random. The naive cost of synthesis and analysis is $\mathcal{O}(n^4)$ but it can be trivially reorganized to $\mathcal{O}(n^3)$ for isolatitude point sets.

Analyzing the error ...

The SH Connection Problem

Theorem 1. Let $\{\phi_n(x)\}_n \geq 0$ and $\{\psi_n(x)\}_{n>0}$ be two families of orthonormal functionss with respect to $L^2(D, d\mu(x))$. Then the connection coefficients satisfy.

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

Any matrix $A \in \mathbb{R}^{m\times n}, m \geq n$, with orthonormal columns is well-conditioned and Moore-Penrose pseudo-invertible $A^+ = A^\top$. For every m, the $\tilde{P}_l^m(x)$ are a family of orthonormal functions for the same Hilbert space $L^2([-1.1].\mathrm{d}x)$

Definition: Let G_n denote the Givens rotation

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

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

idea: 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 $\Rightarrow$ backward stable.
idea: Convert high-order layers to layers of order 0 and 1 in $\mathcal{O}(n^2\log n)$ flops and $\mathcal{O}(n^2\log n)$ storage via the butterfly algorithm; and, Convert low-order layers to Fourier series in $\mathcal{O}(n^2\log n)$ flops and $\mathcal{O}(n\log n)$ storage a la Fast Multipole Method.

Contributions from Sheehan Olver, Alex Townsend, and Mike Clarke
Offers:
1D orthogonal polynomial transforms
Nonuniform fast Fourier transforms
2D harmonic polynomial transforms
Algorithms:
the fast multipole method [Alpert & Rokhlin 1991]
the butterfly algorithm [O'Neil, Woolfe, & Rokhlin 2010]
the fast asymptotic method [Hale & Townsend 2014]
the fast Hadamard product [Townsend, Webb, & Olver 2017]
Indispensable for a reasonably fair comparison.

Contributions from Everett Dawes
Offers:
2D harmonic polynomial transforms
1D orthogonal polynomial transforms (out of necessity)
Algorithms:
Multiple 1D transforms via level-III BLAS
Intel SIMD vectorization (SSE, AVX, AVX-512) of computational kernels
OpenMP parallelization of driver routines
As the mathematically slow algorithms run out of steam, mathematically fast algorithms will be introduced.

5 The Addition Theorem

The spherical harmonic addition thenrem.

$$P_l(x \cdot y) = \frac{4\pi}{2t+1} \sum_{m=-l}^{l} Y_l^m(x) \overline{Y_l^m(y)}$$

shows us that $P_f(x \cdot y)$ is exactly degree l on the sphere. We can use the addition theorem to describe similar expressions. For example, the function:

$$f(z) = \begin{cases} \frac{P_l(z \cdot y) - P_f(x \cdot y)}{z \cdot y - x \cdot y} & \text{for} \quad z \cdot y \neq x \cdot y. \\ P_l'(x \cdot y) & \text{for} \quad z \cdot y = x \cdot y. \end{cases}$$

is in fact a degree $(l-1)$ polynomial on the sphere.
Why the sphere? The unit 2-sphere is the simplest closed bounded surface with genus 0. It has the smallest (constant) curvature-to-volume ratio. It is the starting point to determine if curvature affects the dynamics. It appears in many diverse applications, including cell biology, numerical weather prediction, and astrodynamics. Many partial differential equations of evolution do not need to be accompanied by boundary (volume) conditions on the sphere, which is a major simplification for nonlocal calculus.

Nonlocal diffusion The nonlocal diffusion is:

$$\mathcal{L}_\delta u(x) = \int_{\mathbb{S}^2} \rho_\delta(|x-y|)[u(y)-u(x)]d\Omega(y)$$

where:

$$p_\delta(|x-y|) = \frac{4(1+\alpha)}{\pi\delta^2+2a}\frac{\chi_{[0,\delta]}(|x-y|)}{|x-y|^{2-2n}}$$

is nonnegative and compactly supported by a horizon $0<\delta<2$, and $-1<a<1$ is a parameter governing the strength.
Using the generalized Funk-Hecke formula, we will show:

$$\mathcal{L}_\delta Y_l^m(x) = \lambda_\delta(l) Y_l^m(x)$$

with eigenvalues:

$$\lambda_\delta(l) = 2\pi \int_{1-\delta^2/2}^{1} [P_f(t)-1]\,\rho_\delta(\sqrt{2(1-t)})dt$$

The constants ensure that $\lambda_\delta(l) \to -l(l+1)$ as $\delta \to 0$
Note: generalized Funk-Hecke formula

6 Computation via MCC Quadrature

Modified Clenshaw-Curtis quadrature is exact for degree l polynomials integrands:

$$\int_{-1}^{1} f(x)w(x)\mathrm{d}x = \sum_{k=0}^{l} w_k f\left(x_k\right), \quad \forall f \in \mathbb{P}_\ell$$

The points are $x_k = \cos(k\pi/\ell)$ for $0 \le k \le l$. Using the modified Chebyshev moments:

$$\mu_k = \int_{-1}^{1} T_k(x)w(x)dx, \quad 0 \le k \le l$$

the quadrature weights are obtained via the DCT in $\mathcal{O}(llogl)$. For all $0 \le l \le n$ eigenvalues $\lambda_\delta(l)$, this would cost $\mathcal{O}\left(n^3 \log n\right)$ using the three-term recurrence relation for Legendre polynomials (the integrand). We bring down the cost to $\mathcal{O}\left(n^2 \log n\right)$ by using Szego's asymptotic formula:

$$P_l(\cos\theta) = \sqrt{\frac{\theta}{\sin\theta}} \sum_{\nu=0}^{\infty} \frac{a_\nu(\theta) J_\nu\left(\left(l+\frac{1}{2}\right)\theta\right)}{\left(l+\frac{1}{2}\right)^\nu}$$

Convergence result Sufficiently small time steps $\Rightarrow$ spectral spatial accuracy. Sufficiently large degrees $\Rightarrow$ fourth-order temporal accuracy
It is known that the nonlocal steady-state may be discontinuous, based on the interplay between diffusion strength ϵ and kernel horizon δ.
Note: Why use a spectral method?
A spectral method converges with spectral accuracy arbitrarily close to the discontinuity.

This could be the starting point of a reduced dimension model.
Cesàro ($C.2$) summation as global post-processing removes the Gibbs phenomenon $\Rightarrow$ pointwise convergence almost everywhere.
No better or worse than a finite difference/element/volume method, but the spectrum is trivial.
The double-wrapped Fourier sphere is also popular and synthesis and analysis are fast, but the spectrum is trivial.