COMPUTING ON THE SPHERE PART I: SCALAR HARMONIC ANALYSIS

Paul N. Swarztrauber*

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One of the fundamental differences between spectral analysis on the sphere and rectangle is that vectors on the sphere are discontinuous and require a fundamentally different spectral representation.

For that reason we separate scalar and vector harmonic transforms and begin with scalar transforms of functions such as temperature, pressure, divergence, and vorticity.

TOPICS

Sphere vs rectangle	Least squares representation
Assoc. Legendre fns.	Double Fourier series
Computing the ALFs	Integration formulas
ALFPACK	Gauss points and weights
Scalar harmonic analysis	Generalized harmonic analysis
Aliases and Aliasing	Harmonic projectors
Selecting a finite basis	

*National Center for Atmospheric Research, which is supported by the National Science Foundation, P.O. Box 3000, Boulder, CO 80307

COMPARE SPHERE WITH RECTANGLE

Harmonic analysis is used on a sphere like Fourier analysis on a rectangle but with important differences:

1. Fourier representations are interpolative whereas harmonic representations are approximate in the weighted least squares sense.
2. Discrete Fourier transforms are norm preserving whereas harmonic transforms can magnify.
3. Vector functions are discontinuous (multivalued) at the poles in spherical coordinates.
4. Fourier analysis can be used for both scalar and vector functions on the rectangle. Different analyses are required for scalar and vector functions on the sphere.
5. The FFT can be used for the Fourier transform but not for the Legendre transform.
6. Many terms (not just coefficients) are unbounded in PDEs posed in spherical coordinates.
7. Clustering of grid points near the poles leads to classic "pole problem".
8. $O(N)$ locations are required to store the trigonometric functions whereas $O(N^3)$ locations are required to store the associated Legendre functions $P_n^m(\theta)$ (with notable exceptions).

THE ASSOCIATED LEGENDRE FUNCTIONS

On the sphere, the trigonometric functions are replaced by the modes of the Helmholtz equation (spherical harmonics) $Y_n^m = P_n^m(\theta)e^{im\lambda}$ where θ is colatitude and λ is east longitude.

The $P_n^m(\theta)$ satisfy:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{dP_n^m}{d\theta}) + [n(n+1) - \frac{m^2}{\sin^2\theta}]P_n^m = 0 \qquad (1)$$

With solution given by Rodrigue's formula

$$P_n^m(\theta) = \frac{1}{2^n n!}(\sin\theta)^m \; \frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n \; . \qquad (2)$$

where $x = \cos\theta$.

Rodrigue's formula does not provide a satisfactory method for computing the associated Legendre functions from the standpoint of either speed or accuracy.

The three term recurrence relations are also subject to error near the poles. Consider instead the Fourier method.

THE FOURIER METHOD FOR COMPUTING THE LEGENDRE FUNCTIONS

The Fourier method provides a stable method for computing the associated Legendre functions for any m, n without having to compute the functions for any other m, n.

The differential equation for P_n^m has a solution of the following form that depends on the parity of m and n.

$$P_n^m(\theta) = \sum_{k=0}^{n/2} a_{m,n,k} \cos 2k\theta \qquad n \text{ even}, \quad m \text{ even} \tag{3}$$

$$P_n^m(\theta) = \sum_{k=1}^{n/2} a_{m,n,k} \sin 2k\theta \qquad n \text{ even}, \quad m \text{ odd} \tag{4}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \cos(2k-1)\theta \qquad n \text{ odd}, \quad m \text{ even} \tag{5}$$

$$P_n^m(\theta) = \sum_{k=1}^{(n+1)/2} a_{m,n,k} \sin(2k-1)\theta \qquad n \text{ odd}, \quad m \text{ odd} \tag{6}$$

THE FOURIER METHOD
(continued)

The Fourier representations for $P_n^m(\theta)$ satisfy the differential equation if the $a_{m,n,k}$ satisfy the tridiagonal equations

$$[(2k-1)(2k-2)-n(n+1)]a_{m,n,k-1}-2[4k^2-n(n+1)+2m^2]a_{m,n,k} \\ +[(2k+1)(2k+2)-n(n+1)]a_{m,n,k+1} \;=\; 0\ .$$

The coefficient of $a_{m,n,n/2}$ is zero and the resulting finite number of equations are singular for $m=0,\ldots,n$.

A unique solution is determined by computing $a_{m,n,n/2}$ from Rodrigue's formula and the remaining coefficients by back substitution.

The toughest part is computing $a_{m,n,n/2}$ - more on this later.

Once the $a_{m,n,k}$ are determined the $P_n^m(\theta_i)$ can be tabulated using the quarterwave FFTs from `SPHEREPACK`.

THE RECURRENCE METHOD FOR THE LEGENDRE FUNCTIONS

Using the symmetric FFTs in FFTPACK, the Fourier method requires $O(\log N)$ operations per $P_n^m(\theta_i)$.

However only 4 flops are required using the following four term recurrence relation that is initialized by either P_n^0 or P_n^1 using the Fourier method.

$$\begin{aligned} P_n^m(\theta) &= P_{n-2}^m(\theta) + (n+m-2)(n+m-3)P_{n-2}^{m-2}(\theta) \\ &- (n-m+1)(n-m+2)P_n^{m-2}(\theta) \end{aligned}$$

This recurrence is quite stable in the indicated direction. Indeed the recurrence corresponds to an orthonormal transformation.

P. N. Swarztrauber and W. F. Spotz, Generalized discrete spherical harmonic transforms, *J. Comp. Phys.*, **159**(2000), pp. 213-230.

It does not contain a functional dependence on θ and can therefore be used to compute derivatives, etc.

Because the indices are spaced by 2 the even or odd functions can be computed independently.

All the associated Legendre functions are linear combinations of either P_n^0 or P_n^1.

SOFTWARE FOR COMPUTING THE ASSOCIATED LEGENDRE FUNCTIONS (ALFPACK)

ALFPACK has thirteen user entry points for computing single and double precision, normalized associated Legendre functions of the first kind.

ALFPACK uses the recurrence to tabulate $P_n^m(\theta)$ as a function of either m or n.

ALFPACK contains codes for computing the Fourier coefficients in the trigonometric representations of the Legendre functions

ALFPACK uses the symmetric FFTs to tabulate as a function of θ

ALFPACK contains codes for either a single value of θ or a table of values.

(ACCESSING ALFPACK)

ALFPACK is available via anonymous ftp by executing the command

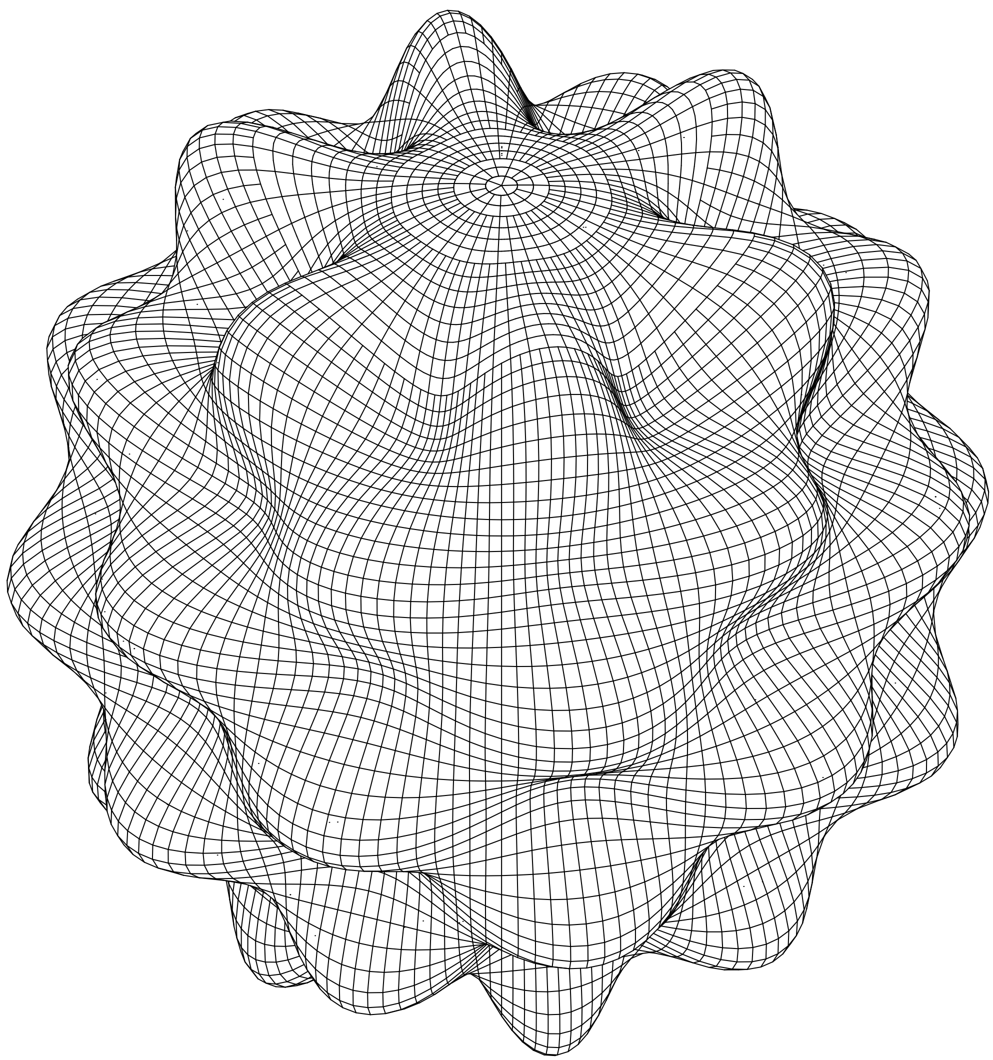
ftp ftp.ucar.edu

Then enter "anonymous" for your name, and your email address for the password. Then follow this session:

```
ftp> cd dsl/lib/alfpack
ftp> mget *
  .
  .  answer y to each question
  .
ftp> quit
```

Back on your host machine, you will have the source code for the entire ALFPACK library, including a makefile.

$\mathbf{Re}[\mathbf{Y}_{12}^{6}(\theta,\lambda)]$



Spherical harmonic, $n = 12, m = 6$ produced by subroutine `visequ` in `spherepack`.

SCALAR HARMONIC ANALYSIS

Given $f_{i,j} = f(\theta_i, \lambda_j)$ we wish to determine complex coefficients $c_{m,n}$ such that:

$$f_{i,j} = \sum_{n=0}^{N} \sum_{m=-n}^{n} c_{m,n} Y_n^m(\theta_i, \lambda_j) \tag{7}$$

where $Y_n^m(\theta_i, \lambda_j)$ are the spherical harmonics

$$Y_n^m(\theta_i, \lambda_j) \;=\; P_n^m(\theta_i) e^{im\lambda_j} \tag{8}$$

The interpolation problem on the sphere does not have a solution!

WHY NOT?

After all - $f_{i,j}$ can be interpolated with a doubly periodic trigonometric series representation .....

More on this later ...

ALIASES

There are only a finite number of e^{ikx} that can be distinguished on a set of points $x_n = n\frac{2\pi}{N}$

$$e^{ink\frac{2\pi}{N}} = e^{-imn2\pi} e^{in(k+mN)\frac{2\pi}{N}} = e^{in(k+mN)\frac{2\pi}{N}} \tag{9}$$

That is: For any k there exists $-N/2 < k_1 \leq N/2$ such that

$$e^{ikx_n} \;=\; e^{ik_1 x_n} \tag{10}$$

Hence e^{ikx} and e^{ik_1x} cannot be distinguished on x_n.

They are alternate characterizations or "aliases" of one another.

Therefore we select the discrete Fourier basis as e^{ikx_n} with the smallest wave numbers $-N/2 < k_1 \leq N/2$.

ALIASING

But what happens if we attempt to interpolate a function with a series representation in terms of more wave numbers than exist in the discrete basis? e.g. assume $f(x)$ has $2N$ coefficients

$$f(x) \;=\; \sum_{k=-N}^{N} c_k \; e^{ikx} \tag{11}$$

On the points x_n the e^{ikx} for $|k| \;>\; N/2$ have aliases in the interval $|k| \;\leq\; N/2$ and

$$f(x_n) \;=\; \sum_{k=0}^{N/2-1} (c_k \;+\; c_{k-N}) \; e^{ink\frac{2\pi}{N}} \tag{12}$$

$$+ \sum_{k=-N/2}^{-1} (c_k \;+\; c_{k+N}) \; e^{ink\frac{2\pi}{N}} \tag{13}$$

Therefore, instead of the c_k a discrete analysis yields

$$c_k \;+\; c_{k-N} \quad \text{for} \quad 0 \;\leq\; k \;\leq\; N/2 \tag{14}$$

$$c_k \;+\; c_{k+N} \quad \text{for} \quad -N/2 \;\leq\; k \;\leq\; -1 \tag{15}$$

The high frequency components $|k| \;>\; N/2$ are said to **alias** onto the low frequency components $|k| \;\leq\; N/2$

We are unable to compute the higher coefficients AND those that we compute are in error.

SELECTING A FINITE DISCRETE BASIS ON THE SPHERE

Recall that $P_n^m(\theta)$ has the Fourier representation

$$P_n^m(\theta) \;=\; \sum_{k=0}^{n/2} a_{m,n,k} \cos 2k\theta \qquad n \text{ even}, \quad m \text{ even} \tag{16}$$

$P_n^m(\theta)$ is included in the discrete basis only if the individual terms in its representation do not have an alias with a smaller wave number. .

For grid with N latitudinal points n must therefore be less than or equal to N. By definition $m \leq n$, which then defines the discrete basis of harmonic functions.

This "triangular truncation" provides an analysis that is invariant under any rotation or translation of the spherical coordinate system. That is, the same harmonic representation is obtained no matter where the pole is placed.

LEAST SQUARES HARMONIC ANALYSIS

On a grid with $2N$ longitudes and N latitudes the discrete harmonic basis consists of the functions

$$\cos m\lambda P_n^m(\theta) \quad \text{and} \quad \sin m\lambda P_n^m(\theta) \tag{17}$$

for $m \leq n$ and $n \leq N$, which yields a total of N^2 basis functions

HOWEVER

this is half the number of grid points $2N^2$, which implies the interpolation problem on the sphere does not have a solution and

Spectral analysis on the sphere is given as the solution to a least squares problem.

P. N. Swarztrauber, On the spectral approximation of discrete scalar and vector functions on the sphere, *SIAM J. Numer. Anal.*, **16**(1979), pp. 934-949.

A CONTRADICTION ?

Any function is doubly periodic on the sphere.

THEREFORE

$a_{m,n}$ can be found such that

$$f_{i,j} = \sum_{n=-N/2}^{N/2} \sum_{m=-N/2}^{N/2} a_{m,n} e^{i(m\theta_i + n\lambda_j)} \quad (18)$$

This would seem to solve the interpolation problem

HOWEVER

The complex exponentials do not provide a satisfactory basis since some are not smooth at the poles.

For example, $e^{i\lambda}$ is discontinuous (multivalued) at the poles and not suitable for the approximation of smooth functions on the sphere.

DOUBLE FOURIER SERIES AND AN IMPORTANT UNSOLVED PROBLEM

Although the double Fourier basis is discontinuous, a number of solvers and methods have been developed using them.... most with the possible exception of

W. F. Spotz, M. A. Taylor, and P. N. Swarztrauber, Fast shallow-water equation solvers in latitude-longitude coordinates, *J. Comp. Phys.*, **145**(1998) pp. 432-444.

The success of this paper is due to the use of a harmonic projection filter that consists of a harmonic analysis followed immediately by a harmonic synthesis.

However the projection slows the method and in some sense defeats the whole purpose of the double Fourier series approach.

Therefore it would be highly desirable to implement the harmonic projection using the double Fourier method.

And of course use the double Fourier method to implement the discrete harmonic transforms themselves.

LEAST SQUARES HARMONIC ANALYSIS
(properties)

Recall that spherical harmonics have representation in terms of homogeneous polynomials in x, y, and z.

Therefore functions are uniformly represented on the sphere independent of the variations in the grid spacing.

e.g. the tabulation $f_{i,j}$ is interpolated at the equator but the points in higher latitudes are progressively smoothed to a greater extent.

Therefore high frequencies that are artificially induced by the closeness of the points near the poles are eliminated.

Model time steps are limited by the distance between points on the equator rather than near the poles.

Unlike aliasing on the rectangle, harmonics of higher degree and order may or may not alias onto an individual harmonic in the discrete basis.

SCALAR HARMONIC ANALYSIS IN THE CONTINUUM

For a real function $f(\theta, \lambda)$ the harmonic analysis consists of determining coefficients $a_{m,n}$ and $b_{m,n}$ such that

$$f(\theta, \lambda) \;=\; \sum_{n=0}^{\infty} \sum_{m=0}^{n} P_n^m(\theta)(a_{m,n} \cos m\lambda \;+\; b_{m,n} \sin m\lambda) \qquad (19)$$

To that end $a_{m,n}$ and $b_{m,n}$ are given by

$$a_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}] \int_0^{2\pi} \int_0^{\pi} f(\theta, \lambda) P_n^m(\theta) \cos m\lambda \cos\theta d\theta d\lambda \qquad (20)$$

$$b_{m,n} \;=\; [\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}] \int_0^{2\pi} \int_0^{\pi} f(\theta, \lambda) P_n^m(\theta) \sin m\lambda \cos\theta d\theta d\lambda \qquad (21)$$

DISCRETE SCALAR HARMONIC ANALYSIS

The longitudinal integrals are approximated with the rectangle rule and computed efficiently using the FFT.

$$a_m(\theta) = \frac{2}{M} \sum_{j=0}^{M-1} f(\theta, \lambda_j) \cos m\lambda_j \tag{22}$$

$$b_m(\theta) = \frac{2}{M} \sum_{j=0}^{M-1} f(\theta, \lambda_j) \sin m\lambda_j \tag{23}$$

then

$$a_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}] \int_0^\pi a_m(\theta) P_n^m(\theta) \cos\theta d\theta \tag{24}$$

$$b_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}] \int_0^\pi b_m(\theta) P_n^m(\theta) \cos\theta d\theta \tag{25}$$

How are the latitudinal integrals computed?

LATITUDINAL QUADRATURES

Current weather/climate models use Gauss-Legendre quadrature with weights w_i and points θ_i

$$a_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N-1} w_i P_n^m(\theta_i) a_m(\theta_i) \qquad (26)$$

$$b_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N-1} w_i P_n^m(\theta_i) b_m(\theta_i) \qquad (27)$$

The Machenhauer-Daley (MD) quadrature provides the same accuracy on equally spaced points $\theta_i = i\pi/M$

$$a_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N} Z_n^m(\theta_i) a_m(\theta_i) \qquad (28)$$

$$b_{m,n} = [\frac{2n+1}{2\pi}\frac{(n-m)!}{(n+m)!}]\sum_{i=0}^{N} Z_n^m(\theta_i) b_m(\theta_i) \qquad (29)$$

LATITUDINAL QUADRATURES
(continued)

1. The $Z_n^m(\theta)$ are selected so the quadrature is exact for any $Y_n^m(\theta, \lambda)$ in the finite basis.

2. These seemingly different quadrature formulas will be unified and generalized to an arbitrary set θ_i on a later slide.

3. However, for now we note only that the $Z_n^m(\theta)$ have the same "form" in the forward transform as the $P_n^m(\theta)$ in the backward transform.

4. Although the Gauss and equally spaced quadratures provide the same accuracy, they alias differently...

5. Software is available in SPHEREPACK for both Gauss and equally spaced distribution of points.

REPRESENTING A VECTOR IN TERMS OF A GIVEN SET OF VECTORS

Given an arbitrary set of vectors $\mathbf{A}$ then

$$\mathbf{A}^{\mathrm{T}}(\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1}\mathbf{A} = \mathbf{I} \tag{30}$$

where for the moment we ignore the fact that the inverse may not exist.

If we define $\mathbf{W} = (\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1}$ then the vectors $\mathbf{A}$ are weighted orthogonal in the sense that $\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{A} = \mathbf{I}$.

Given an arbitrary vector $\mathbf{f}$ then $\mathbf{f} = \mathbf{A}\mathbf{a}$ where $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$, which provides the representation of $\mathbf{f}$ in terms of the vectors $\mathbf{A}$.

Now $\mathbf{W}^{-1} = \mathbf{A}\mathbf{A}^{\mathrm{T}}$ is symmetric positive semidefinite with decomposition $\mathbf{W}^{-1} = \mathbf{U}\mathbf{S}^2\mathbf{U}^{\mathrm{T}}$ where $\mathbf{U}$ is orthogonal (eigenvectors of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$) $\mathbf{S}^2$ is diagonal (eigenvalues of $\mathbf{A}\mathbf{A}^{\mathrm{T}}$). Therefore

$$\mathbf{A}^{\mathrm{T}}\mathbf{U}\mathbf{S}^{-2}\mathbf{U}^{\mathrm{T}}\mathbf{A} = \mathbf{I}\ . \tag{31}$$

Therefore $\mathbf{V}^{\mathrm{T}} = \mathbf{S}^{-1}\mathbf{U}^{\mathrm{T}}\mathbf{A}$ is orthogonal and yields the singular value decomposition of an arbitrary matrix $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{T}}$.

REPRESENTING A FUNCTION IN TERMS OF OF A GIVEN SET OF FUNCTIONS

The vectors $\mathbf{A}$ on the previous slide were arbitrary and can therefore be tabulations of arbitrary functions on an arbitrary set of points. In this manner any tabulation $\mathbf{f}$ can be expressed in terms of the functions selected to determine $\mathbf{A}$ by $\hat{\mathbf{f}} = \mathbf{Aa}$ where

$$\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} \tag{32}$$

or in terms of the SVD

$$\mathbf{a} = \mathbf{V}\mathbf{S}^{-1}\mathbf{U}^{\mathrm{T}}\mathbf{f} \tag{33}$$

Note that

$$\mathbf{W} = (\mathbf{A}\mathbf{A}^{\mathrm{T}})^{-1} = \mathbf{U}\mathbf{S}^{-2}\mathbf{V}^{\mathrm{T}} \tag{34}$$

Therefore (33) would be preferred to (32) because of its superior conditioning.

However, for a large class of basis functions on a prescribed set of points one can often develop closed form representations for computing $\mathbf{a}$. e.g. Gauss and equally spaced point distributions.

This also provides formulas for computing the approximation of derivatives, integrals or a host of other derived quantities.

GENERALIZED LEGENDRE TRANSFORMS

We now turn to a specific example of the general theory developed above. Define $\mathbf{A}$ to be the Legendre polynomials tabulated on an arbitrary latitudes θ_i.

We now replace the arbitrary vectors $\mathbf{A}$ with the Legendre polynomials tabulated on an arbitrary set of latitudes θ_i.

$$\mathbf{A} = \begin{bmatrix} P_0(\theta_1) & \cdots & P_{N-1}(\theta_1) \\ \vdots & \ddots & \vdots \\ P_0(\theta_N) & \cdots & P_{N-1}(\theta_N) \end{bmatrix}, \tag{35}$$

The Christoffel-Darboux formula yields the following elements of $\mathbf{W}^{-1}$.

$$(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{i,j} = \frac{N}{\sqrt{4N^2-1}} \frac{P_N(\theta_i)P_{N-1}(\theta_j) - P_{N-1}(\theta_i)P_N(\theta_j)}{\cos\theta_i - \cos\theta_j}. \tag{36}$$

The diagonal elements can be computed directly from $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ or from l'Hôpital's rule.

$$(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{i,i} = \frac{N}{\sqrt{4N^2-1}\cos\theta_i} \left[P_{N-1}(\theta_i)\frac{d}{d\theta}P_N(\theta_i) - P_N(\theta_i)\frac{d}{d\theta}P_{N-1}(\theta_i) \right]. \tag{37}$$

GENERALIZED LEGENDRE TRANSFORMS
(continued)

In this manner the transform $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ generalizes the Legendre transform to an arbitrary set of latitudes and in the process, unifies Gauss and equally spaced latitudinal points θ_i.

If the θ_i are selected as the zeros of $P_N(\theta_i)$ then $\mathbf{W}$ is diagonal and the resulting θ_i are known as the Gaussian Legendre points and the $(\mathbf{W})_{i,i}$ are the Gaussian weights.

Note that this does not save compute time because the transform $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ still requires multiplication by $\mathbf{A}^{\mathrm{T}}$.

We turn now to the computation of the points and weights corresponding to Gauss-Legendre quadrature.

COMPUTING GAUSS-LEGENDRE POINTS

Recall that $P_n(\theta)$ has the Fourier representation

$$P_n(\theta) = \sum_{k=0}^{n} a_{n,k} \cos k\theta \,, \tag{38}$$

For $m = 0$ the tridiagonal equations for the coefficients $a_{m,n,k}$ reduce to the bidiagonal set of equations

$$[n(n+1)-k(k+1)]a_{n,k}+[(k+1)(k+2)-n(n+1)]a_{n,k+2} = 0. \tag{39}$$

The coefficient of $a_{n,n}$ is zero and therefore $a_{n,n}$ can be arbitrary. If we specify

$$a_{n,n} = \sqrt{\frac{2n+1}{2}}\frac{1\cdot 3\cdot 5\cdots(2n-1)}{2^{n-1}n!} = \sqrt{\frac{2n+1}{2}}\frac{\Gamma(2n+1)}{2^{2n-1}\Gamma^2(n+1)} \tag{40}$$

The resulting coefficients $a_{n,k}$ yield the normalized Legendre polynomials.

- $a_{n,n}$ can be difficult to compute because the Γ function will quickly overflow as a function of n.
- Instead we observe that $a_{n,n}$ is a smooth bounded function of $y = 1/n$ on the interval $[0, 1]$ that can be computed in 10 to 12 flops using a rational approximation.

COMPUTING GAUSS-LEGENDRE POINTS
(continued)

- Given its Fourier representation, the zeros of $P_n(\theta)$ or Gauss-Legendre points can now be computed using Newtons method.

- Near the equator the points are almost equally spaced. This provides a sufficiently accurate initial guess that only a single Newton iteration is required.

- Subsequent initial estimates are obtained by linear extrapolation of previous points. In practice, only a few of the points at the end of the interval require an additional Newton iteration.

A method for computing the points and weights is presented in "Computing the points and weights for Gauss-Legendre quadrature", *SIAM J. Sci. Comput.*, **24**(2002) pp. 945-954.

COMPUTING GAUSS-LEGENDRE WEIGHTS

Using the three point recurrence satisfied by the Legendre polynomials and the fact that $P_n(\theta_i) = 0$ we obtain the following equivalent formulas for the Gauss-Legendre weights.

$$w_i^{(a)} = -\frac{\sqrt{(2n-1)(2n+1)}\cos\theta_i}{n\bar{P}_{n-1}(\theta_i)\bar{P}_n'(\theta_i)} \qquad w_i^{(b)} = \frac{(2n-1)\cos^2\theta_i}{n^2\bar{P}_{n-1}^2(\theta_i)}$$

$$w_i^{(c)} = \frac{\sqrt{(2n+1)(2n+3)}\cos\theta_i}{(n+1)\bar{P}_{n+1}(\theta_i)\bar{P}_n'(\theta_i)} \qquad w_i^{(d)} = \frac{(2n+3)\cos^2\theta_i}{(n+1)^2\bar{P}_{n+1}^2(\theta_i)}$$

$$w_i^{(e)} = -\frac{\sqrt{(2n-1)(2n+3)}\cos^2(\theta_i)}{n(n+1)\bar{P}_{n-1}(\theta_i)\bar{P}_{n+1}(\theta_i)} \qquad w_i^{(f)} = \frac{2n+1}{\left[\bar{P}_n'(\theta_i)\right]^2}.$$

- Although analytically identical - they differ computationally in the sense that only $w_i^{(f)}$ provides relative as well as absolute accuracy.
- The methods for computing Gauss points and weights have been implemented in subroutine `gaqd` in `spherepack` and tested to a million points in single precision.
- The points can be computed to machine precision for any n; however, the error growth in the weights is proportional to n.

GENERALIZED DISCRETE SPHERICAL HARMONIC TRANSFORMS

Here we summarize the results from Swarztrauber and Spotz, Generalized spherical harmonic transforms, *J. Comp. Phys.*, **159**(2000) pp. 213-230.

1. The Legendre transforms are generalized to an arbitrary latitudinal distribution of points thereby unifying the transforms based on Gauss and equally spaced distribution as well as providing new transforms for other grid distributions used to model geophysical processes.

2. Memory efficient alternative Legendre transforms are developed whose coefficients in spectral space are rotations of the traditional spectral coefficients. These transforms require $\mathcal{O}(N^2)$ memory compared to the traditional $\mathcal{O}(N^3)$.

3. Faster transforms are developed based on the alternative Legendre transforms and their orthogonal complement. A computational savings of up to 50% can be realized.

The speed and accuracy of several projection methods are given by Spotz and Swarztrauber in:

A performance comparison of associated Legendre projections, *J. Comp. Phys.*, **168**(2001) pp. 339-355.

SPHERICAL HARMONIC PROJECTORS

- Using the simplified notation developed earlier we define the forward transform into spectral space or harmonic analysis as $\mathbf{a} = \mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f}$ where $\mathbf{f}$ is the tabulation of some scalar function on the surface of the sphere. The transform back into physical space or harmonic synthesis is given by $\hat{\mathbf{f}} = \mathbf{A}\mathbf{a}$. Hence the projector is given by $\mathbf{P} = \mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}$.

- The forward followed by the backward transform can be subject to considerable error (or not exist) depending on the distribution of latitudinal points θ_i.

- This problem disappears if the projections are computed using the singular value decomposition $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{T}}$

$$\mathbf{W} = \mathbf{U}\mathbf{S}^{-2}\mathbf{U}^{\mathrm{T}} \quad \text{and} \quad \mathbf{P} = \mathbf{U}\mathbf{U}^{\mathrm{T}}. \tag{41}$$

- It is evident that $\mathbf{W}$ can be very ill conditioned (because of the factor $\mathbf{S}^{-2}$). However $\mathbf{P}$ is well conditioned (actually best possible) for any distribution of points θ_i.

- The attractive stability and accuracy of spectral transform method for weather and climate simulations result from the harmonic projectors that are explicit or implicit to these models.

SPHERICAL HARMONIC PROJECTORS
(Summary)

Here we summarize the results from Swarztrauber and Spotz, Spherical harmonic projectors, which will appear in *Math. Comp.*.

Variant spherical harmonic projections are defined with the following attributes.

1. The variant projection is norm preserving in the l_2 sense, unlike the traditional spherical harmonic projection.
2. On a Gaussian grid the singular values of the variant projectors are up to 10 percent less than the traditional analysis matrix.
3. The error associated with the variant projection is marginally less than the traditional projection on a Gauss distributed latitudinal grid but may be substantially less on an arbitrary grid.
4. The variant projections are symmetric and expressed as the outer product of orthonormal vectors from a single $N \times N$ matrix compared with traditional projections that require N such matrices.
5. The algorithm for computing the variant projections, as well as the projections themselves, are well conditioned for any latitudinal grid distribution.

LEAST SQUARES - IN WHAT NORM ?

Given $f_{i,j}$ both Gauss and MD quadratures determine $a_{m,n}$ and $b_{m,n}$ such that

$$\hat{f}_{i,j} = \sum_{n=0}^{N-1} \sum_{m=0}^{n} P_n^m(\theta_i)(a_{m,n} \cos m\lambda_j + b_{m,n} \sin m\lambda_j) \tag{42}$$

is a least squares approximation to $f_{i,j}$.

The continuous norm is:

$$||f(\theta,\lambda)||^2 = \frac{1}{2\pi}\int_0^{2\pi} \int_0^{\pi} f^2(\theta,\lambda)\cos\theta d\theta d\lambda \tag{43}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{n} a_{m,n}^2 = \mathbf{a}^{\mathrm{T}}\mathbf{a} \tag{44}$$

THE DISCRETE NORM

The continuous norm suggests the following discrete norm

$$\| \mathbf{f} \|_{\mathbf{W}} = \mathbf{a}^{\mathrm{T}}\mathbf{a} = \mathbf{f}^{\mathrm{T}}\mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} = \mathbf{f}^{\mathrm{T}}\mathbf{W}\mathbf{f} \qquad (45)$$

1. This discrete norm with $\mathbf{W} = \mathbf{U}\mathbf{S}^{-2}\mathbf{V}^{\mathrm{T}}$ is exact for any Y_n^m in the discrete basis (otherwise a pseudo norm).

2. $\hat{f}_{i,j} = \mathbf{P}\mathbf{f} = \mathbf{A}\mathbf{A}^{\mathrm{T}}\mathbf{W}\mathbf{f} = \mathbf{U}\mathbf{U}^{\mathrm{T}}\mathbf{f}$ is a weighted least squares approximation to $f_{i,j}$ in the $\mathbf{W}$ norm

3. $\hat{f}_{i,j}$ provides a uniform approximation to $f_{i,j}$ that is independent of the coordinate system and consequently eliminates the high frequencies that can be induced by the closeness of points near the poles.