Spherical harmonics

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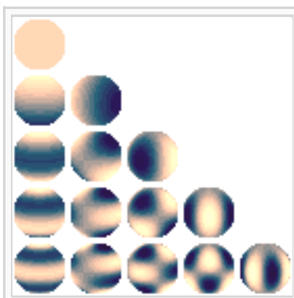
In mathematics, the **spherical harmonics** are the angular portion of an orthogonal set of solutions to Laplace's equation represented in a system of spherical coordinates. Spherical harmonics are important in many theoretical and practical applications, particularly in the computation of atomic electron configurations, representation of gravitational fields, geoids, and the magnetic fields of planetary bodies, and characterization of the cosmic microwave background radiation. In 3D computer graphics, spherical harmonics plays a special role in a wide variety of topics including indirect lighting (ambient occlusion, global illumination, precomputed radiance transfer etc) and in recognition of 3D shapes.

Contents

Introduction

Laplace's equation in spherical coordinates is:



Real spherical harmonics Y_{lm}, for l=0 to 4 (top to bottom) and m=0 to 4 (left to right). The negative order harmonics $Y_{l\text{-}m}$ are rotated about the z axis by 90/m degrees with respect to the positive order ones.

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2} = 0$$

(see also del in cylindrical and spherical coordinates). For $f(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$, the angular portion of Laplace's equation satisfies

$$\frac{\Phi(\varphi)}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{\Theta(\theta)}{\sin^2\theta}\frac{d^2\Phi}{d\varphi^2} + l(l+1)\Theta(\theta)\Phi(\varphi) = 0.$$

Using the technique of separation of variables, two differential equations result:

$$\frac{1}{\Phi(\varphi)}\frac{d^2\Phi(\varphi)}{d\varphi^2} = -m^2$$

$$l(l+1)\sin^2(\theta) + \frac{\sin(\theta)}{\Theta(\theta)}\frac{d}{d\theta}\left[\sin(\theta)\frac{d\Theta}{d\theta}\right] = m^2$$

for some m and l. Hence, the angular solutions can be shown to be a products of trigonometric functions and associated Legendre functions:

$$Y_\ell^m(\theta,\varphi) = N\, e^{im\varphi}\, P_\ell^m(\cos\theta),$$

where Y_ℓ^m is a called a spherical harmonic function of degree ℓ and order m, P_ℓ^m is an associated Legendre function, N is a normalization constant, and θ and ϕ represent colatitude and longitude, respectively. The spherical coordinates used in this article are consistent with those used by physicists, but differ from those employed by mathematicians (see spherical coordinates). In particular, the colatitude θ, or polar angle, ranges from $0 \le \theta \le \pi$ and the longitude ϕ, or azimuth, ranges from $0 \le \phi \le 2\pi$. Thus, θ is 0 at the North Pole, $\pi/2$ at the Equator, and π at the South Pole.

When Laplace's equation is solved on the surface of the sphere, the periodic boundary conditions in ϕ, as well as regularity conditions at both the north and south poles, ensure that the degree ℓ and order m are integers that satisfy $\ell \ge 0$ and $|m| \le \ell$. In contrast, if the function f were only to have been defined for $\theta \le \theta_0$, then the resulting spherical cap harmonics would have been defined for integer order, but non-integer degree. The general solution to Laplace's equation is a linear combination of the spherical harmonic functions multiplied by the solutions of $R(r)$:

$$f(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} r^{-1-\ell}\, f_\ell^m\, Y_\ell^m(\theta,\varphi) + \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} r^{\ell}\, f_\ell^{m'}\, Y_\ell^m(\theta,\varphi),$$

where f_ℓ^m and $f_\ell^{m'}$ are constants. The terms in the first summation approach zero as r goes to infinity, whereas the terms in the second summation approach zero at the origin.

Orthogonality and normalization

Several different normalizations are in common use for the spherical harmonic functions. In physics and seismology, these functions are generally defined as

$$Y_\ell^m(\theta,\varphi) = \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\varphi}$$

which are orthonormal

$$\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} Y_\ell^m\, Y_{\ell'}^{m'*}\, d\Omega = \delta_{\ell\ell'}\,\delta_{mm'},$$

where $\delta_{aa} = 1$, $\delta_{ab} = 0$ if $a \neq b$, (see Kronecker delta) and $d\Omega = \sin\theta\, d\phi\, d\theta$. The disciplines of geodesy and spectral analysis use

$$Y_\ell^m(\theta,\varphi) = \sqrt{(2\ell+1)\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\varphi}$$

which possess unit power

$$\frac{1}{4\pi}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} Y_\ell^m\, Y_{\ell'}^{m'*} d\Omega = \delta_{\ell\ell'}\,\delta_{mm'}.$$

The magnetics community, in contrast, uses Schmidt semi-normalized harmonics

$$Y_\ell^m(\theta,\varphi) = \sqrt{\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\varphi}$$

which have the normalization

$$\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} Y_\ell^m\, Y_{\ell'}^{m'*} d\Omega = \frac{4\pi}{(2\ell+1)}\delta_{\ell\ell'}\,\delta_{mm'}.$$

In quantum mechanics this normalization is often used, too, and is there named Racah's normalization after Giulio Racah.

Using the identity (see associated Legendre functions)

$$P_\ell^{-m} = (-1)^m \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m$$

it can be shown that all of the above normalized spherical harmonic functions satisfy

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

where the superscript * denotes complex conjugation. Alternatively, this equation follows from the relation of the spherical harmonic functions with the Wigner D-matrix.

Condon-Shortley phase

One source of confusion with the definition of the spherical harmonic functions concerns a phase factor of $(-1)^m$, commonly referred to as the Condon-Shortley phase in the quantum mechanical literature. In the quantum mechanics community, it is common practice to either include this phase factor in the definition of the associated Legendre functions, or to append it to the definition of the spherical harmonic functions. There is no requirement to use the Condon-Shortley phase in the definition of the spherical harmonic functions, but including it can simplify some quantum mechanical operations, especially the application of raising and lowering operators. The geodesy and magnetics communities never include the Condon-Shortley phase factor in their definitions of the spherical harmonic functions.

Spherical harmonics expansion

The spherical harmonics form a complete set of orthonormal functions and thus form a vector space analogous to unit basis vectors. On the unit sphere, any square-integrable function can thus be expanded as a linear combination of these:

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

This expansion is exact as long as ℓ goes to infinity. Truncation errors will arise when limiting the sum over ℓ to a finite bandwidth L. The expansion coefficients can be obtained by multiplying the above equation by the complex conjugate of a spherical harmonic, integrating over the solid angle Ω, and utilizing the above orthogonality relationships. For the case of orthonormalized harmonics, this gives:

$$f_\ell^m = \int_\Omega f(\theta,\varphi)\, Y_\ell^{m*}(\theta,\varphi) d\Omega = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta f(\theta,\varphi) Y_\ell^{m*}(\theta,\varphi).$$

An alternative set of spherical harmonics for real functions may be obtained by taking the set:

$$Y_{\ell m} = \begin{cases} Y_\ell^0 & \text{if } m = 0 \\ \frac{1}{\sqrt{2}}\left(Y_\ell^m + (-1)^m\, Y_\ell^{-m}\right) = \sqrt{2} N_{(l,m)} P_\ell^m(\cos\theta)\cos m\varphi & \text{if } m > 0 \\ \frac{1}{i\sqrt{2}}\left(Y_\ell^{-m} - (-1)^m\, Y_\ell^{m}\right) = \sqrt{2} N_{(l,m)} P_\ell^{-m}(\cos\theta)\sin m\varphi & \text{if } m < 0. \end{cases}$$

where $N_{(l,m)}$ denotes the normalization constant as a function of l and m. These functions have the same normalization properties as the complex ones above. In this notation, a real square-integrable function can be expressed as an infinite sum of real spherical harmonics as:

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

See here for a list of real spherical harmonics up to and including $l = 5$. Note, however, that the listed functions differ by the phase $(-1)^m$ from the phase given in this article.

Spectrum analysis

The total power of a function f is defined in the signal processing literature as the integral of the function squared, divided by the area it spans. Using the orthonormality properties of the real unit-power spherical harmonic functions, it is straightforward to verify that the total power of a function defined on the unit sphere is related to its spectral coefficients by a generalization of Parseval's theorem:

$$\frac{1}{4\,\pi}\int_\Omega f(\Omega)^2\, d\Omega = \sum_{l=0}^{\infty} S_{ff}(l),$$

where

$$S_{ff}(l) = \sum_{m=-l}^{l} f_{lm}^2$$

is defined as the angular power spectrum. In a similar manner, one can define the cross-power of two functions as

$$\frac{1}{4\,\pi}\int_\Omega f(\Omega)\, g(\Omega)\, d\Omega = \sum_{l=0}^{\infty} S_{fg}(l),$$

where

$$S_{fg}(l) = \sum_{m=-l}^{l} f_{lm} g_{lm}$$

is defined as the cross-power spectrum. If the functions f and g have a zero mean (i.e., the spectral coefficients f_{00} and g_{00} are zero), then $S_{ff}(l)$ and $S_{fg}(l)$ represent the contributions to the function's variance and covariance for degree ℓ, respectively. It is common that the (cross-)power spectrum is well approximated by a power law of the form

$$S_{ff}(l) = C\,\ell^{\beta}.$$

When $\beta = 0$, the spectrum is "white" as each degree possesses equal power. When $\beta < 0$, the spectrum is termed "red" as there is more power at the low degrees with long wavelengths than higher degrees. Finally, when $\beta > 0$, the spectrum is termed "blue".

Addition theorem

A mathematical result of considerable interest and use is called the *addition theorem* for spherical harmonics. Two vectors **r** and **r'**, with spherical coordinates (r, θ, φ) and (r', θ', φ'),respectively, have an angle γ between them given by

$$\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi').$$

The addition theorem expresses a Legendre polynomial of order *l* in the angle γ in terms of products of two spherical harmonics with angular coordinates (θ, φ) and (θ', φ'):

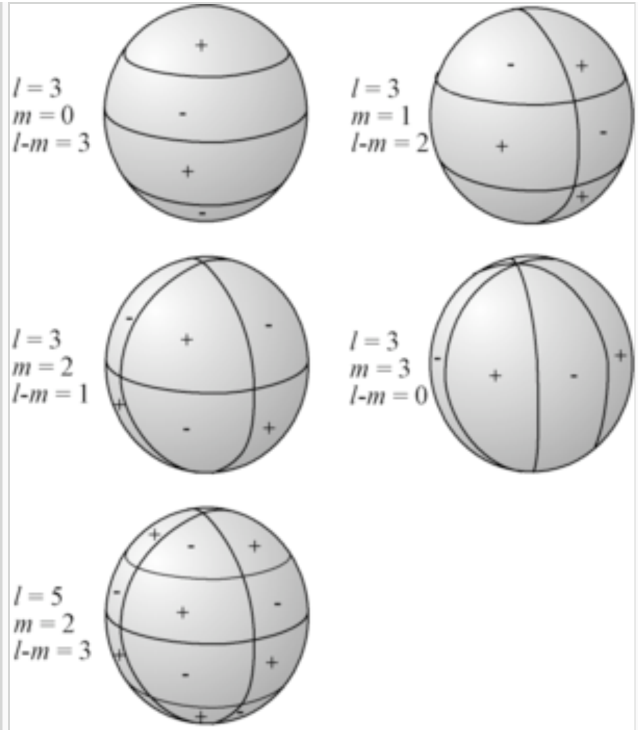
$$P_l(\cos\gamma) = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_{lm}^{*}(\theta', \varphi')\,Y_{lm}(\theta, \varphi).$$

This expression is valid for both real and complex harmonics. However, it should be emphasized that the quoted form above is valid only for the orthonormalized spherical harmonics. For unit power harmonics it is only necessary to remove the factor of 4π.

Visualization of the spherical harmonics

The spherical harmonics are easily visualized by counting

The spherical harmonics are easily visualized by counting the number of zero crossings they possess in both the latitudinal and longitudinal directions. For the latitudinal direction, the associated Legendre functions possess $l - |m|$ zeros, whereas for the longitudinal direction, the trigonomentric sin and cos functions possess $2|m|$ zeros.



Schematic representation of Y_{lm} on the unit sphere. Y_{lm} is equal to 0 along m great circles passing through the poles, and along l-m circles of equal latitude. The function changes sign each time it crosses one of these lines.

When the spherical harmonic order m is zero, the spherical harmonic functions do not depend upon longitude, and are referred to as **zonal**. When $l = |m|$, there are no zero crossings in latitude, and the functions are referred to as **sectoral**. For the other cases, the functions checker the sphere, and they are referred to as **tesseral**.

First few spherical harmonics

Analytic expressions for the first few orthonormalized spherical harmonics that use the Condon-Shortley phase convention:

$$Y_0^0(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{1}{\pi}}$$

$$Y_1^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\,\sin\theta\,e^{-i\varphi}$$

$$Y_1^0(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\,\cos\theta$$

$$Y_1^1(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{3}{2\pi}}\,\sin\theta\,e^{i\varphi}$$

$$Y_2^{-2}(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\,e^{-2i\varphi}$$

$$Y_2^{-1}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\theta\,\cos\theta\,e^{-i\varphi}$$

$$Y_2^0(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\,(3\cos^2\theta - 1)$$

$$Y_2^1(\theta,\varphi) = \frac{-1}{2}\sqrt{\frac{15}{2\pi}}\,\sin\theta\,\cos\theta\,e^{i\varphi}$$

$$Y_2^2(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\,e^{2i\varphi}$$

$$Y_3^0(\theta,\varphi) = \frac{1}{4}\sqrt{\frac{7}{\pi}}\,(5\cos^3\theta - 3\cos\theta)$$

More spherical harmonics up to $\mathbf{Y_{10}}$

Generalizations

The spherical harmonics map can be seen as representations of the symmetry group of rotations around a point (SO(3)) and its double-cover SU(2). As such they capture the symmetry of the two-dimensional sphere (or two-sphere). Each set of spherical harmonics with a given value for the l-parameter map onto a different irreducible representation of SO(3).

In addition, the two-sphere is equivalent to the Riemann sphere. The complete set of symmetries of the Riemann sphere are described by the Möbius transformation group PSL(2,C), which is isomorphic as a real Lie group to the Lorentz group. The analog of the spherical harmonics for the Lorentz group are given by the hypergeometric series; indeed, the spherical harmonics can be re-expressed in terms of the hypergeometric series, as SO(3) is a subgroup of PSL(2,C).

More generally, hypergeometric series can be generalized to describe the symmetries of any symmetric space; in particular, hypergeometric series can be developed for any Lie group[1][2][3][4]

Slater integrals or coefficients

John C. Slater defined the integral of three spherical harmonics as a coefficient *c* [5]

$$c^k(l,m,l,'m') = \int d^2\Omega\ Y_l^m(\Omega)^* Y_{l'}^{m'}(\Omega) Y_k^{m-m'}(\Omega)$$

These integrals are useful and necessary when doing atomic calculations of the Hartree-Fock variety where matrix elements of the Coulomb operator are needed. For an explicit formula, one can use Gaunt's formula under the section on Associated Legendre functions.

These coefficient obey a number of identities. They include

$$\begin{aligned} c^k(l,m,l',m') &= c^k(l,-m,l',-m') \\ &= (-1)^{m-m'} c^k(l',m',l,m) \\ &= (-1)^{m-m'} \sqrt{\frac{2l+1}{2k+1}} c^l(l',m',k,m'-m) \\ &= (-1)^{m'} \sqrt{\frac{2l'+1}{2k+1}} c^{l'}(k,m-m',l,m) \end{aligned}$$

$$\sum_{m=-l}^{l} c^k(l,m,l,m) = (2l+1)\delta_{k,0}$$

$$\sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} c^k(l,m,l',m')^2 = \sqrt{(2l+1)(2l'+1)} \cdot c^k(l,0,l',0)$$

$$\sum_{m=-l}^{l} c^k(l,m,l',m')^2 = \sqrt{\frac{2l+1}{2l'+1}} \cdot c^k(l,0,l',0)$$

$$\sum_{m=-l}^{l} c^k(l,m,l',m') c^k(l,m,\tilde{l},m') = \delta_{l',\tilde{l}} \cdot \sqrt{\frac{2l+1}{2l'+1}} \cdot c^k(l,0,l',0)$$

$$\sum_{m} c^k(l,m+r,l',m) c^k(l,m+r,\tilde{l},m) = \delta_{l,\tilde{l}} \cdot \frac{\sqrt{(2l+1)(2l'+1)}}{2k+1} \cdot c^k(l,0,l',0)$$

$$\sum_{m} c^k(l,m+r,l',m) c^q(l,m+r,l',m) = \delta_{k,q} \cdot \frac{\sqrt{(2l+1)(2l'+1)}}{2k+1} \cdot c^k(l,0,l',0)$$

See also

- Clebsch-Gordan coefficients
- Harmonic function
- Rotation group
- Sturm-Liouville theory
- Atomic orbital
- Solid harmonics
- Vector spherical harmonics
- Table of spherical harmonics

References

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2. ^ J. D. Talman, *Special Functions, A Group Theoretic Approach*, (based on lectures by E.P. Wigner), W. A. Benjamin, New York (1968).
3. ^ W. Miller, *Symmetry and Separation of Variables,* Addison-Wesley, Reading (1977).
4. ^ A. Wawrzyńczyk, *Group Representations and Special Functions*, Polish Scientific Publishers. Warszawa (1984).
5. ^ John C. Slater, Quantum Theory of Atomic Structure, McGraw-Hill (New York, 1960), Volume I

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Web resources

- Spherical harmonics on Mathworld (http://mathworld.wolfram.com/SphericalHarmonic.html)
- Spherical Harmonic Models of Planetary Topography (http://www.ipgp.jussieu.fr/~wieczor/SH/SH.html)
- Spherical harmonics generator in OpenGL (http://adomas.org/shg/)
- OpenGL Spherical harmonics demo (http://www.paulsprojects.net/opengl/sh/sh.html)

Software

- SHTOOLS: Fortran 95 software archive (http://www.ipgp.jussieu.fr/~wieczor/SHTOOLS/SHTOOLS.html)
- HEALPIX: Fortran 90 and C++ software archive (http://healpix.jpl.nasa.gov/)
- SpherePack: Fortran 77 software archive (http://www.cisl.ucar.edu/css/software/spherepack/)
- SpharmonicKit: C software archive (http://www.cs.dartmouth.edu/~geelong/sphere/)
- Frederik J Simons: Matlab software archive (http://geoweb.princeton.edu/people/simons/software.html)
- NFFT: C subroutine library (fast spherical Fourier transform for arbitrary nodes) (http://www-user.tu-chemnitz.de/~potts/nfft/)
- Shansyn: spherical harmonics package for GMT/netcdf grd files (http://www.spice-rtn.org/library/software/shansyn)
- SHAPE: Spherical HArmonic Parameterization Explorer (http://www.embl-heidelberg.de/~khairy/links.html)

External links

- Interactive calculator of spherical harmonics on [http://wm.eecs.umich.edu:8180/webMathematica/tcarmon/sh2.jsp Tal Carmon's Research Homepage
- Spherical harmonics applied to Acoustic Field analysis on Trinnov Audio's research page (http://www.trinnov.com/research.php#concept)
- Spherical Harmonics (http://demonstrations.wolfram.com/SphericalHarmonics/) by Stephen Wolfram and Nodal Domains of Spherical Harmonics (http://demonstrations.wolfram.com/NodalDomainsOfSphericalHarmonics/) by Michael Trott, The Wolfram Demonstrations Project
- An accessible introduction to spherical harmonics (by J. B. Calvert) (http://mysite.du.edu/~jcalvert/math/harmonic/harmonic.htm)
- Spherical harmonics entry at Citizendium (http://en.citizendium.org/wiki/Spherical_harmonics)

Categories: Partial differential equations | Special hypergeometric functions | Atomic physics | Fourier analysis | Geophysics | Rotational symmetry