Spherical Harmonics

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Abstract Spherical harmonics are special functions that can be used to contruct representations of the rotation group. This article presents an easy way to construct all spherical harmonics in D-dimensional space for any $D \geq 3$, without using spherical coordinates.

Contents

1 Notation

A point in D-dimensional euclidean space will be denoted

$$\mathbf{x} = (x_1,\, ...,\, x_D).$$

The gradient with respect to $\mathbf{x}$ will be denoted

$$\nabla = (\nabla_1,\, ...,\, \nabla_D)$$

where ∇_k is the partial derivative with respect to x_k:

$$\nabla_k \equiv \frac{\partial}{\partial x_k}.$$

The abbreviations

$$r \equiv |\mathbf{x}| \qquad\qquad \mathbf{u} \equiv \frac{\mathbf{x}}{r}$$

will be used, and the identity $\mathbf{x}\cdot\nabla r^n = nr^n$ is often useful. When the number of spatial dimensions is $D = 3$, subscripts will be avoided by using the notation

$$\mathbf{x} = (x,\, y,\, z)$$

for the components of $\mathbf{x}$.

Throughout this article, the word **operator** is used as an abbreviation for *differential operator*. For two operators A and B, the standard notation

$$[A, B] \equiv AB - BA$$
$$\{A, B\} \equiv AB + BA$$

will be used. These are called the **commutator** and **anticommutator**, respectively.

2 The generators of rotations

The operator

$$L_{jk} \equiv x_j \nabla_k - x_k \nabla_j \tag{1}$$

satisfies

$$L_{jk}\, r = 0.$$

We can think of L_{jk} as the derivative with respect to an angle, namely the angle about the **origin** (the point $\mathbf{x} = 0$) in the j-k plane.

The operator L_{jk} **generates** rotations about the origin in the j-k plane, in this sense: for any function $f(\mathbf{x})$, the new function

$$f_\phi(\mathbf{x}) \equiv \exp(\phi L_{jk}) f(\mathbf{x}) \tag{2}$$

is a rotated version of the original, with rotation angle ϕ. To prove this, use the abbreviations $c \equiv \cos\phi$ and $s \equiv \sin\phi$, and consider the function

$$f_\phi(\mathbf{x}) = f(cx_1 - sx_2,\, sx_1 + cx_2,\, x_3,\, x_4,\, ...). \tag{3}$$

This function clearly satisfies

$$f_{\phi=0}(\mathbf{x}) = f(\mathbf{x}), \tag{4}$$

and it also satisfies

$$\frac{d}{d\phi} f_\phi(\mathbf{x}) = L_{12}\, f_\phi(\mathbf{x}) \tag{5}$$

because both sides are equal to

$$(-sx_1 - cx_2) f_1 + (cx_1 - sx_2) f_2$$

where f_n is the derivative of the right-hand side of (3) with respect to its nth argument. Equations (4)-(5) are the definition of the right-hand side of (2) when $j, k = 1, 2$. The same idea works for other index-pairs j, k, too. This completes the proof.

Since L_{jk} generates rotations about the origin, a function $f(\mathbf{x})$ is invariant under rotations about the origin if and only if $L_{jk} f = 0$ for all j, k. In particular, $L_{jk} r = 0$.

3 An invariant combination of generators

The operators L_{jk} don't commute with each other, but they all commute with the operator

$$\mathbf{L}^2 \equiv \frac{1}{2}\sum_{j,k} L_{jk}^2. \tag{6}$$

To prove this, start with the fact that two L_{jk}s fail to commute only when they have exactly one subscript in common,[1] such as L_{12} and L_{23}. Use the definition (1) to confirm the identity

$$[L_{12}, (L_{23})^2] = \{L_{13}, L_{23}\}.$$

Permute subscript-values to get

$$[L_{12}, (L_{13})^2] = -[L_{21}, (L_{13})^2] = -\{L_{23}, L_{13}\}.$$

Two results together imply $[L_{12}, \mathbf{L}^2] = 0$. The general case

$$[L_{jk}, \mathbf{L}^2] = 0 \tag{7}$$

follows by permuting the subscripts.

[1] For $D \geq 4$, some L_{jk}s don't have any subscripts in common, like L_{12} and L_{34}. Such L_{jk}s commute with each other, which should be obvious from the definition (1).

4 Spherical harmonics: motivation

Let $Y(\mathbf{x})$ denote a function that is defined for all $r > 0$ and that satisfies the conditions

$$\boxed{\mathbf{x}\cdot\nabla Y = 0 \qquad\qquad \mathbf{L}^2 Y \propto Y.} \tag{8}$$

Here's some intuition about these conditions:

- The first condition says that Y is invariant under $\mathbf{x} \to \kappa\mathbf{x}$ for all $\kappa \neq 0$. In other words, it says that Y depends only on angles about the origin – that is, only on the unit vector $\mathbf{u} \equiv \mathbf{x}/r$. We can think of Y as a function defined on the surface of the unit sphere.[2]

- The second condition in (8) says that Y is an **eigenfunction** of $\mathbf{L}^2$. The proportionality factor is called the **eigenvalue**. The operators L_{jk} generate rotations about the origin (section 2), so equation (7) implies that eigenfunctions of $\mathbf{L}^2$ with different eigenvalues don't mix with each other under rotations about the origin.

When seeking solutions $f(\mathbf{x})$ of a rotation-symmetric partial differential equation, the ansatz $f(\mathbf{x}) = \rho(r)Y(\mathbf{x})$ is often helpful. The first condition in (8) says that the factor $\rho(r)$ accounts for all of the r-dependence, and the second condition in (8) says something about how the solution transforms under rotations.

The conditions (8) are often used as the definition of the class of functions called *spherical harmonics*. This article uses a different but equivalent definition, introduced in section 6.

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[2]Such functions can also be described using **spherical coordinates**. Spherical coordinates have the virtue of being non-redundant (the number of coordinates is the same as the number of dimensions of the surface of the sphere), but they are not defined at all points on the surface of the sphere, and they obscure spherical symmetry: the way they transform under rotations is a horrific mess. Using $\mathbf{x}/r$ to parameterize the unit sphere is often easier, even though it's redundant (it uses D coordinates, whereas the surface of the unit sphere has only $D-1$ dimensions), because $\mathbf{x}/r$ is defined everywhere on the unit sphere and transforms in a very simple way (namely linearly) under all rotations about the origin.

5 Harmonic polynomials

Spherical harmonics will be defined in terms of special polynomials called harmonic polynomials. A polynomial $g(\mathbf{x})$ in the components of $\mathbf{x}$ is called **homogeneous** if

$$g(\kappa\mathbf{x}) = \kappa^\ell g(\mathbf{x}) \tag{9}$$

for some nonnegative integer ℓ called the **degree** of the polynomial. This implies

$$\mathbf{x}\cdot\nabla g = \ell g. \tag{10}$$

A **harmonic polynomial** is a homogeneous polynomial $h(\mathbf{x})$ that satisfies

$$\nabla^2 h = 0. \tag{11}$$

The differential operator

$$\nabla^2 \equiv \sum_k \nabla_k^2$$

is called the **laplacian**. This notation will be used:

- P_ℓ is the vector space[3] of homogeneous polyonomials of degree ℓ.
- $H_\ell \subset P_\ell$ is the vector space[3] of harmonic polyomials of degree ℓ.

In both cases, the number of real variables is understood to be D, the number of components of $\mathbf{x}$.

[3] This is a vector space because any linear combination of such polynomials is another such polynomial.

6 Spherical harmonics: definition

A **spherical harmonic of degree** ℓ is a function of the form

$$\boxed{Y(\mathbf{x}) = \frac{h(\mathbf{x})}{r^\ell} \qquad\qquad \text{with } h \in H_\ell.} \tag{12}$$

Section (7) derives equations (8) as consequences of the definition (12). The converse can also be proved: the conditions (8) imply (12).[4]

Using the definition (12), section 8 highlights a relatively easy way to construct spherical harmonics, and sections 9-10 show that every spherical harmonic is a linear combination of those.

[4]This is part (1) of theorem 1.9 in Gallier (2013), section 1.4, page 28.

7 Derivation of (8) from (12)

The laplacian can be expressed in terms of the operators $\mathbf{x}\cdot\nabla$ and L_{jk}, which are derivatives in radial and angular directions, respectively. Explicitly,

$$r^2\nabla^2 = (D-2+\mathbf{x}\cdot\nabla)\mathbf{x}\cdot\nabla + \mathbf{L}^2. \tag{13}$$

To derive this, use the definitions (1) and (6) to evaluate $\mathbf{L}^2$ in terms of ∇^2 and $\mathbf{x}\cdot\nabla$. By the way, the same result may be written in terms of $\mathbf{u}\cdot\nabla$ instead of $\mathbf{x}\cdot\nabla$. To do this, use the identity

$$(\mathbf{x}\cdot\nabla)^2 = r^2(\mathbf{u}\cdot\nabla)^2 + \mathbf{x}\cdot\nabla$$

to get

$$\nabla^2 = \left(\frac{D-1}{r} + \mathbf{u}\cdot\nabla\right)\mathbf{u}\cdot\nabla + \frac{1}{r^2}\mathbf{L}^2. \tag{14}$$

This version might be more familiar than (13).

The goal is to prove that any function of the form (12) satisfies both of the conditions (8). The first condition in (8) is equivalent to invariance under $\mathbf{x}\to\kappa\mathbf{x}$, so the fact that (12) satisfies the first condition in (8) is clear from the fact that h is homogeneous (equation (9)). To show that function (12) also satisfies the second condition in (8), use equations (10), (11), and (13) to get

$$\mathbf{L}^2 h = -\ell(\ell+D-2)\,h,$$

and combine this with $L_{jk}\,r = 0$ to get[5]

$$\mathbf{L}^2\,Y = -\ell(\ell+D-2)\,Y. \tag{15}$$

This shows that Y satisfies the second condition in (8). This completes the proof.

[5] When $D=3$, equation (15) reduces to $\mathbf{L}^2\,Y = -\ell(\ell+1)Y$, a result highlighted in many introductions to quantum mechanics.

8 Constructing harmonic polynomials

Suppose $D \geq 3$.[6] Then, for any list of ℓ indices $a, b, c, ...$, the function

$$h(\mathbf{x}) = r^{2\ell+D-2}\, \nabla_a \nabla_b \nabla_c \cdots \frac{1}{r^{D-2}} \tag{16}$$

is a harmonic polynomial of degree ℓ. The fact that it is a polynomial of degree ℓ should be clear by inspection. This section shows that it also satisfies the harmonic condition 11.[7]

Use the abbreviation

$$s \equiv \nabla_a \nabla_b \nabla_c \cdots \frac{1}{r^{D-2}}, \tag{17}$$

with ℓ gradients, so that equation (16) becomes

$$h(\mathbf{x}) = r^{2\ell+D-2}\, s.$$

Start with the identity

$$\nabla^2 h = r^{2\ell+D-2} \nabla^2 s + s \nabla^2 r^{2\ell+D-2} + 2(\nabla r^{2\ell+D-2}) \cdot \nabla s. \tag{18}$$

The first term on the right-hand side is zero because $\nabla^2(1/r^{D-2}) = 0$ for all $r > 0$. To evaluate the second term on the right-hand side of (18), use

$$\begin{aligned} \nabla^2 r^{2\ell+D-2} &= (2\ell + D - 2)\nabla \cdot (\mathbf{x} r^{2\ell+D-4}) \\ &= (2\ell + D - 2)(D + 2\ell + D - 4) r^{2\ell+D-4}. \end{aligned}$$

To evaluate the third term on the right-hand side of (18), use

$$\begin{aligned} (\nabla r^{2\ell+D-2}) \cdot (\nabla s) &= (2\ell + D - 2) r^{2\ell+D-4} \mathbf{x} \cdot \nabla s \\ &= (2\ell + D - 2)(2 - D - \ell) r^{2\ell+D-4} s. \end{aligned}$$

Combine these intermediate results to get the final result $\nabla^2 h = 0$.

[6] For $D = 2$, use $\log r$ in place of $1/r^{D-2}$.

[7] This is lemma 5.15 on page 86 in Axler *et al* (2020), also expressed in words on page 85.

9 Completeness

If $D \geq 3$, then every harmonic polynomial of degree ℓ can be written as a linear combination of polynomials of the form (16). This is proved in Axler *et al* (2020). Here's an outline:[8]

- Given a function $u(\mathbf{x})$ defined for all $r > 0$, its **Kelvin transform**[9] is defined to be $r^{2-D}u(\mathbf{x}/r^2)$. In particular, the Kelvin transform of the function (17) is the function (16).[10]

- If $p(\mathbf{x})$ is a polynomial, then the polynomial $r^2p(\mathbf{x})$ cannot be harmonic.[11]

- If $\ell \geq 2$, then every polynomial in P_ℓ can be written[12] $p(\mathbf{x}) = h(\mathbf{x}) + r^2p'(\mathbf{x})$, where $h \in H_\ell$ and $p' \in P_{\ell-2}$, and this decomposition is unique.[13] This defines the **canonical projection** of the space of homogeneous polynomials into the space of harmonic polynomials.

- If $D \geq 3$, then the Kelvin transform of any linear combination of functions of the form 17 is proportional to the canonical projection of the same linear combination of the corresponding monomials $x_a x_b x_c \cdots$ (using the same index-values) into the space of harmonic polynomials.[14]

- Altogether, this implies[15] that every every harmonic polynomial of degree ℓ can be written as a linear combination of polynomials of the form (16).

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[8] This outline is based on Axler *et al* (2020), which is available on-line for free. A similar proof is given in Vilenkin (1968), chapter 9.

[9] Axler *et al* (2020), pages 59 and 61

[10] This can be deduced without calculating the gradients. Just use the fact that (17) is a homogeneous polynomial of degree ℓ (in the components of $\mathbf{x}$) divided by $r^{2-D+2\ell}$.

[11] Axler *et al* (2020), corollary 5.3 on page 75, and Vilenkin (1968), chapter 9, section 2, page 444

[12] Axler *et al* (2020), proposition 5.5 on page 76

[13] Axler *et al* (2020), page 76. Vilenkin (1968) says it this way (chapter 9, section 2, page 444): if $\ell \geq 2$, then P_ℓ is the **direct sum** of H_ℓ and $r^2P_{\ell-2}$.

[14] Axler *et al* (2020), theorem 5.18 on page 88

[15] Axler *et al* (2020), page 92.

10 Constructing spherical harmonics

Combining (12) and (16) to get

$$\boxed{Y(\mathbf{x}) = r^{\ell+D-2}\,\nabla_a\nabla_b\nabla_c\cdots\frac{1}{r^{D-2}} \qquad \text{(with } \ell \text{ gradients).}} \tag{19}$$

The results in sections 8-9 imply that when $D \geq 3$, every spherical harmonic of degree ℓ is a linear combination of these.

For $D \geq 3$, the function $1/r^{D-2}$ satisfies

$$\nabla^2\frac{1}{r^{D-2}} = 0 \qquad \text{for } r > 0.$$

For $D = 2$, the corresponding relationship is $\nabla^2 \log r = 0$ for $r > 0$. Replacing $1/r^{D-2}$ with $\log r$ in the formula (19) gives spherical harmonics for $D = 2$. This article is mostly concerned with $D \geq 3$.

11 Examples

Up to proportionality, there is one spherical harmonic of degree $\ell = 0$, namely $Y \propto 1$. For degrees $\ell > 0$, straightforward evaluation of derivatives gives

$$\begin{aligned}
\nabla_a \frac{1}{r^{D-2}} &= (2-D)\frac{x_a}{r^D} \\
\nabla_a \nabla_b \frac{1}{r^{D-2}} &= (2-D)\frac{\delta_{ab} r^2 - D x_a x_b}{r^{D+2}} \\
\nabla_a \nabla_b \nabla_c \frac{1}{r^{D-2}} &= (2-D)D\frac{(2+D)x_a x_b x_c - (x_a\delta_{bc} + x_b\delta_{ca} + x_c\delta_{ab})r^2}{r^{D+4}}
\end{aligned}$$

and so on. Therefore, according to the formula (19), the spherical harmonics for the first few degrees $\ell = 1, 2, 3$ are

$$\begin{aligned}
Y_a(\mathbf{u}) &\propto \frac{x_a}{r} \\
Y_{ab}(\mathbf{u}) &\propto \frac{D x_a x_b - \delta_{ab} r^2}{r^2} \\
Y_{abc}(\mathbf{u}) &\propto \frac{(2+D)x_a x_b x_c - (x_a\delta_{bc} + x_b\delta_{ca} + x_c\delta_{ab})r^2}{r^3}.
\end{aligned}$$

The number of linearly independent spherical harmonics is shown below for the first few degrees ℓ:

ℓ	# lin indep	# lin indep when $D = 3$
0	1	1
1	D	3
2	$(D^2 + D - 2)/2$	5
3	$(D^3 + 3D^2 - 4D)/6$	7

The general result is given as a function of D and ℓ in Axler *et al* (2020), proposition 5.8 on page 78.

12 Examples for $D = 3$

Equation (8) says that spherical harmonics are eigenfunctions of $\mathbf{L}^2$. We may choose a basis for the set of spherical harmonics so that each basis function is also an eigenfunction of L_{12}, because L_{12} commutes with $\mathbf{L}^2$ (section 3). When $D = 3$, the eigenvalues of $\mathbf{L}^2$ and L_{12} specify the function completely, up to proportionality.

In this section, set $D = 3$ and let $Y_{\ell,m}$ denote a spherical harmonic of degree ℓ that satisfies

$$L_{12}Y_{\ell,m} = im\,Y_{\ell,m}.$$

For the first few degrees ℓ, the solutions are[16]

$$\begin{aligned}
\ell = 0:&\quad Y_{00} \propto 1\\
\ell = 1:&\quad r\;Y_{11} \propto x + iy\\
&\quad r\;Y_{10} \propto z\\
\ell = 2:&\quad r^2\;Y_{22} \propto (x + iy)^2\\
&\quad r^2\;Y_{21} \propto (x + iy)z\\
&\quad r^2\;Y_{20} \propto 3z^2 - r^2\\
\ell = 3:&\quad r^3\;Y_{33} \propto (x + iy)^3\\
&\quad r^3\;Y_{32} \propto (x + iy)^2 z\\
&\quad r^3\;Y_{31} \propto (x + iy)(5z^2 - r^2)\\
&\quad r^3\;Y_{30} \propto (5z^2 - 3r^2)z
\end{aligned}$$

together with $Y_{\ell,-m} = Y^*_{\ell m}$. To construct $Y_{\ell m}$ for any ℓ and any $m \geq 0$, start with

$$r^\ell\;Y_{\ell m} \propto (x + iy)^m\;h(z, r^2)$$

where $h(z, r^2)$ is a homogeneous polynomial of order $\ell - m$ in z and r with only even powers of r. This automatically satisfies $\partial_\phi Y_{\ell m} = im\;Y_{\ell m}$. Now just solve

$$\nabla^2(r^\ell\;Y_{\ell m}) = 0$$

for the integer coefficients in the polynomial $h(z, r^2)$.

[16] In this section, the components of $\mathbf{x}$ are written as (x, y, z) instead of (x_1, x_2, x_3). The functions displayed here are often written in terms of angles ϕ and θ defined by $x + iy = r\;\exp(i\phi)$ and $z = r\;\cos\theta$.

13 Representations of the rotation group

The group of rotations about the origin in D-dimensional space is the **special orthogonal group** $SO(D)$.[17] In a **representation** of the rotation group on a vector space V, each rotation acts as a linear transformation of V (article 29682).

When V is the vector space H_ℓ of harmonic polynomials of degree ℓ, we have a natural representation in which the effect of a rotation R on $h(\mathbf{x}) \in H_\ell$ is[18]

$$h(\mathbf{x}) \to h(R\mathbf{x}), \tag{20}$$

where

$$\mathbf{x} \to R\mathbf{x} \tag{21}$$

is the usual effect of a rotation on $\mathbf{x}$. Using the definition (12), this gives an equivalent representation of the rotation group on the vector space of spherical harmonics of degree ℓ, because the denominator in (12) is invariant under (21).

[17] The **orthogonal group** $O(D)$ also includes reflections.

[18] This transformation preserves the degree ℓ because (21) is linear, and it preserves the harmonic condition (11) because the laplacian ∇^2 is invariant under (21).

14 Are the representations irreducible?

A representation of a group on a vector space V is called **irreducible** if V does not have any nontrivial subspace that is self-contained under the action of the group. According to Vilenkin (1968), the representation of $SO(D)$ on H_ℓ defined by (20) is irreducible if $D \geq 3$. Vilenkin (1968) doesn't quite say that directly, but it's implied by these statements from Vilenkin (1968), chapter 9, section 2, where the proofs are worked out in detail:[19,20]

- Page 441: $SO(D)$ acts irreducibly on the quotient space $P_\ell/r^2 P_{\ell-2}$.
- Page 445: The representation of $SO(D)$ on $P_\ell/r^2 P_{\ell-2}$ is equivalent to its representation on H_ℓ.

Altogether, this says that the representation defined by (20) is irreducible, and therefore so is the equivalent representation on the space of spherical harmonics of degree ℓ.

[19] These statements don't specify any restriction on D, but the restriction $D \geq 3$ is acknowledged on pages 452-453 in the same section.

[20] The page numbers refer to Vilenkin (1968).

15 Other irreducible representations

$SO(D)$ has other irreducible representations that are not equivalent to any of the representations defined by (20) on the space of harmonic polynomials (or spherical harmonics). Any homogeneous polynomial of degree ℓ may be written

$$\sum_{a,b,c,\ldots} A_{abc\cdots} x_a x_b x_c \cdots \qquad \text{(with } \ell \text{ indices)}, \tag{22}$$

where the coefficients $A_{abc\cdots}$ are complex numbers. Applying a rotation R to the coordinates, as in (21), is the same as applying the transformation

$$A_{abc\cdots} \to \sum_{a',b',c',\ldots} A_{a'b'c'\cdots} R_{a'a} R_{b'b} R_{c'c} \cdots \tag{23}$$

to the coefficients, where R_{ab} is the rotation matrix defined by $(Rx)_a = \sum_b R_{ab} x_b$. A representation defined by (20) corresponds to a representation defined by (23) with special constraints on the coefficients. We can get new irreducible representations of the form (23) by imposing different constraints on the coefficients. Some of them are equivalent to one of the representations defined by (20), but some are not.[21]

An example is the representation of $SO(D)$ on the set of antisymmetric matrices, $A_{ab} = -A_{ba}$. The corresponding polynomials (22) are zero, but the transformations (23) still define a nontrivial representation of $SO(D)$, one that is not expressed in terms of polynomials. For $D = 3$, this antisymmetric representation doesn't give us anything new: it's equivalent to the representation defined by (20) with $\ell = 1$ (article 81674). In contrast, for $D = 4$, it does give us something new. It gives a reducible representation containing two irreducible subrepresentations, in which the coefficients satisfy either of the additional constraints $A_{ab} = \pm \sum_{cd} \epsilon_{abcd} A_{cd}$, where ϵ_{abcd} is completely antisymmetric. These are often called the **self-dual** and **anti-self-dual** representations, respectively. Neither one of them is equivalent to any of the representations defined by (20).

[21] Fulton and Harris (1991) introduces a systematic approach to constructing all irreducible representations of a finite-dimensional Lie group on finite-dimensional real and complex vector spaces. The case of $SO(D)$ is addressed in theorem 19.22 and chapter 26.

16 References

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