The Laplacian in polar coordinates and spherical harmonics

These notes present the basics about the Laplacian in polar coordinates, in any number of dimensions, and attendant information about circular and spherical harmonics, following in part Taylor's book [Ta].

1. The Laplacian in polar coordinates. We introduce general polar coordinates on $\mathbb{R}^n$, with $n \ge 2$, by writing $r = \sqrt{x_1^2 + \cdots + x_n^2}$ and $\theta = (\theta_1, \ldots, \theta_{n-1})$. The most important cases are $n = 2$ and $n = 3$, but the cases $n \ge 4$ are also important in more advanced work. If $n = 2$ we write more simply $\theta_1 = \theta$ and have

$$x_1 = r\cos\theta, \qquad x_2 = r\sin\theta, \tag{1}$$

If $n = 3$ one usually writes something like

$$x_1 = r\sin\theta_1\cos\theta_2, \qquad x_2 = r\sin\theta_1\sin\theta_2, \qquad x_3 = r\cos\theta_1, \tag{2}$$

but this involves choosing x_3 as a preferred axis and so it is good to postpone this choice and leave $(\theta_1, \ldots, \theta_{n-1})$ unspecified at first.

Returning to the case $n \ge 2$ arbitrary, we compute the effect of the Laplacian $\Delta = \partial_{x_1}^2 + \cdots \partial_{x_n}^2$ on a function in product form $u(r)v(\theta)$ as follows:

$$\Delta(uv) = (\Delta u)v + 2\nabla u \cdot \nabla v + u\Delta v = (\Delta u)v + u\Delta v.$$

For the first equals sign, we used the general product rule $(uv)_{x_jx_j} = u_{x_jx_j}v + 2u_{x_j}v_{x_j} + uv_{x_jx_j}$. For the second one, we used the fact that the coordinates r and θ are orthogonal: $\nabla f \cdot \nabla g = 0$ because ∇f is perpendicular to S_r and ∇g is tangent to S_r, where S_r is the sphere centered at 0 with radius r.

We compute Δu using the chain rule: since $r = \sqrt{x_1^2 + \cdots + x_n^2}$ we have

$$\partial_{x_j}u(r) = u'(r)\partial_{x_j}r = u'(r)x_j/r,$$

and computing similarly $\partial_{x_j}^2 u(r)$ and summing in j gives

$$\Delta u(r) = u''(r) + \tfrac{n-1}{r}u'(r).$$

Hence

$$\Delta(uv) = (\partial_r^2 + \tfrac{n-1}{r}\partial_r + \Delta_{S_r})(uv),$$

where Δ_{S_r} denotes the angular derivatives in Δ, i.e. it is defined by the equation $\Delta_{S_r}(uv) = u\Delta v$ for any functions $u = u(r)$ and $v = v(\theta)$.

We can simplify this expression further by relating S_r to S_1 by scaling. If $c > 0$ and $\Delta f = g$, then by the chain rule $\Delta f(cx) = c^2 g(cx)$. That means $\Delta_{S_r} = r^{-2}\Delta_{S_1}$, leading us to the formula

$$\Delta_{\mathbb{R}^n} = \partial_r^2 + \tfrac{n-1}{r}\partial_r + \tfrac{1}{r^2}\Delta_{\mathbb{S}^{n-1}}. \tag{3}$$

To compute $\Delta_{\mathbb{S}^{n-1}}$, the Laplacian on the unit sphere, more explicitly, we need to specify the θ coordinates. In the key cases (1), (2) we have respectively

$$\Delta_{\mathbb{S}^1} = \partial_\theta^2, \qquad \Delta_{\mathbb{S}^2} = \partial_{\theta_1}^2 + \cot\theta_1\partial_{\theta_1} + \csc^2\theta_1\partial_{\theta_2}^2.$$

But below we extract information from (3) without using any formula for $\Delta_{\mathbb{S}^{n-1}}$.

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2. Homogeneous harmonic polynomials. A polynomial is homogeneous of degree ℓ if each of its terms has degree exactly ℓ. For example $x_1^3x_2 + x_3^4$ is homogeneous of degree 4, but $x_1^3x_2 + x_3^3$ is not homogeneous. Such a polynomial is harmonic if its Laplacian is zero. For example $x_1^2 - x_2^2$ is harmonic but $x_1^2 + x_2^2$ is not.

Let $p(r,\theta) = r^\ell v(\theta)$ be a homogeneous harmonic polynomial of degree ℓ. Then

$$0 = \Delta p = \ell(\ell-1)r^{\ell-2}v(\theta) + \ell(n-1)r^{\ell-2}v(\theta) + r^{\ell-2}\Delta_{\mathbb{S}^{n-1}}v(\theta).$$

Simplifying yields

$$-\Delta_{\mathbb{S}^{n-1}}v(\theta) = \ell(\ell+n-2)v(\theta).$$

Thus v is an eigenvector of $\Delta_{\mathbb{S}^{n-1}}$ with eigenvalue $\ell(\ell+n-2)$. It is a remarkable fact that *all* the eigenvalues and eigenvectors of $\Delta_{\mathbb{S}^{n-1}}$ are obtained in this way. The eigenvectors are called spherical harmonics in general, and circular harmonics when $n=2$. Let us examine them one dimension at a time.

3. Circular harmonics. If $n=2$, then $\ell(\ell+n-2)=\ell^2$, and using $\Delta_{\mathbb{S}^1} = \partial_\theta^2$ we see right away that the corresponding space of eigenvectors is spanned by $\{1\}$ if $\ell = 0$ and by $\{\cos \ell\theta, \sin\ell\theta\}$ if $\ell \neq 0$.

We can also replace use of the formula $\Delta_{\mathbb{S}^1} = \partial_\theta^2$ with computation of harmonic polynomials, because this method works well for $n \geq 3$ as well.

We begin by writing some bases for the sets of homogeneous polynomials of degree ℓ. These are $\{1\}$, $\{x_1, x_2\}$, $\{x_1^2, x_1x_2, x_2^2\}$, $\dots$, $\{x_1^\ell, x_1^{\ell-1}x_2, \dots, x_2^\ell\}, \dots$.

If $\ell = 0$ or $\ell = 1$ then they are all harmonic, and so writing $x_1 = r\cos\theta$ and $x_2 = r\sin\theta$ we get the bases $\{1\}$ and $\{\cos\theta, \sin\theta\}$ for the corresponding circular harmonics.

If $\ell \geq 2$, then we compute the harmonic ones by writing

$$0 = \Delta\sum_{k=0}^{\ell} a_k x_1^{\ell-k}x_2^k = \sum_{k=0}^{\ell-2} a_k(\ell-k)(\ell-k-1)x_1^{\ell-k-2}x_2^k + \sum_{k=2}^{\ell} a_k k(k-1)x_1^{\ell-k}x_2^{k-2}.$$

Matching coefficients gives

$$0 = a_k(\ell-k)(\ell-k-1) + a_{k+2}(k+2)(k+1). \tag{4}$$

Thus a_0 and a_1 may be chosen freely, and after that the other a_k are determined by (4). Hence the space of harmonic homogeneous polynomials of degree ℓ has dimension 2. We can find a basis for this space by writing

$$0 = \Delta(x_1 + ix_2)^\ell$$

and taking the real part as one basis vector and the imaginary part as the other. The formulas in terms of x_1 and x_2 are complicated (they come from Pascal's triangle and can be written in terms of binomial coefficients) but the formulas in terms of θ are very nice: we write

$$(x_1 + ix_2)^\ell = r^\ell e^{i\ell\theta} = r^\ell(\cos\ell\theta + i\sin\ell\theta)$$

and see that a basis is $\{\cos\ell\theta, \sin\ell\theta\}$.

4. Spherical harmonics. If $n=3$, then $\ell(\ell+n-2) = \ell(\ell+1)$, It is not so easy to find the spherical harmonics using the formula for $\Delta_{\mathbb{S}^2}$. It can be done using Legendre polynomials: see Section 5.4 of [Bo].

In terms of harmonic polynomials, we can compute the bases as follows. If $\ell = 0$ or $\ell = 1$, as before we have respectively $\{1\}$ and $\{x_1, x_2, x_3\}$.

If $\ell = 2$, we write

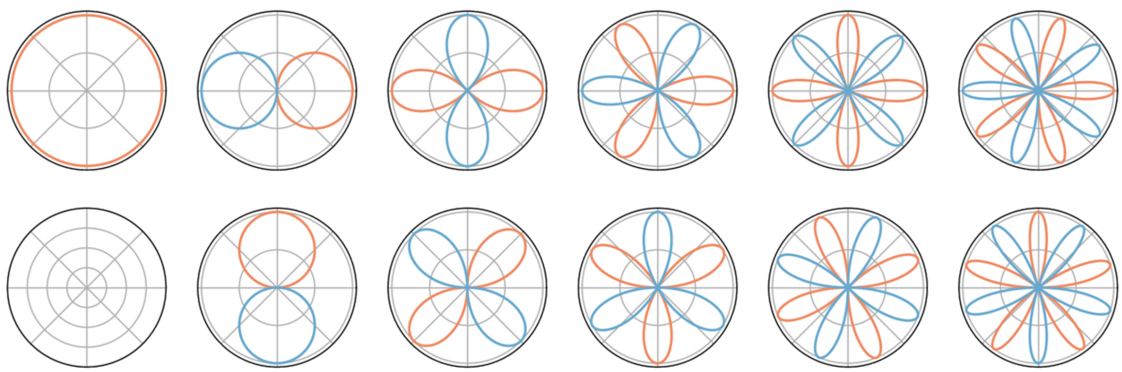
$$0 = \Delta(a_0x_1^2 + a_1x_2^2 + a_2x_3^2 + a_3x_1x_2 + a_4x_2x_3 + a_5x_1x_3) = a_0 + a_1 + a_2.$$

Eliminating a_0, we see that a general homogeneous harmonic polynomial of degree 2 can be written

$$a_1(x_2^2 - x_1^2) + a_2(x_3^2 - x_1^2) + a_3x_1x_2 + a_4x_2x_3 + a_5x_1x_3,$$

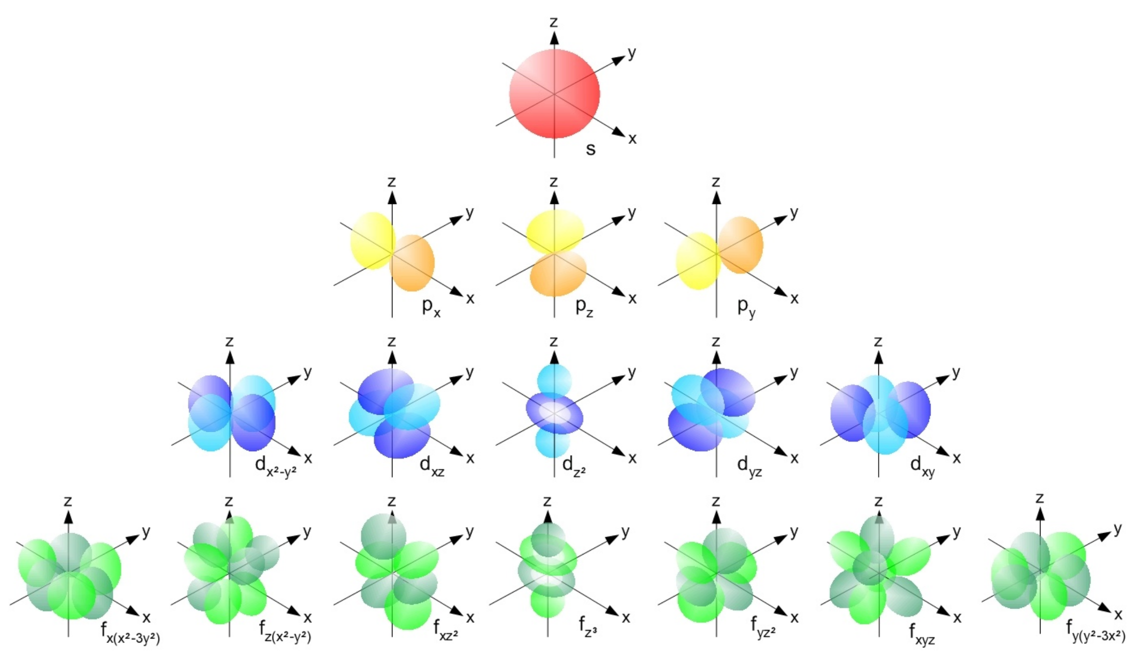
and thus a basis is $\{x_2^2 - x_1^2,\, x_3^2 - x_1^2,\, x_1x_2,\, x_2x_3,\, x_1x_3\}$.

5. Pictures. Here is a picture of circular harmonics, from `https://mkofinas.github.io/post/circ_harmonics/`:



Above, the first column shows $\ell = 0$, the second column shows $\ell = 1$, etc. Orange denotes positive values, and blue denotes negative. The distance to the origin denotes the magnitude of the function. Thus the first function is constant and positive, the second is positive on the right and negative on the left, with a maximum at $\theta = 0$, a minimum at $\theta = \pi$, and zeroes at $\theta = \pm\pi/2$.

Spherical harmonics are most famous as orbitals of electrons. Here is a picture from `https://no.wikipedia.org/wiki/Fil:Single_electron_orbitals.jpg`.



Above, the first row is $\ell = 0$, the second row is $\ell = 1$, etc.

Note that if $n = 2$, then the dimension of each eigenspace is 2 unless $\ell = 0$ in which case the dimension is 1. If $n = 3$, then the dimension of each eigenspace is $2\ell+1$. Thus higher values of ℓ are no more complicated than lower values of ℓ if $n = 2$, but they are significantly more complicated if $n = 3$, and even moreso as n increases.

6. Going deeper. Note that if $n = 2$, then the dimension of each eigenspace is 2 unless $\ell = 0$ in which case the dimension is 1. If $n = 3$, then the dimension of each eigenspace is $2\ell + 1$. Thus higher values of ℓ are no more complicated than lower values of ℓ if $n = 2$, but they are significantly more complicated if $n = 3$, and even moreso as n increases. The computation of dimension for general ℓ and n, including the proof that no eigenspaces are omitted by the method above, is in Section 7.4 of [Ta].

The labels of the pictures of orbitals match the bases of eigenfunctions found in Section for $\ell = 0$ and $\ell = 1$, but for $\ell = 2$ there is a discrepancy: the picture for z^2 does not match the basis element $x_3^2 - x_1^2$. This is because that because for orbitals one uses a special basis of eigenfunctions: one uses a basis of joint eigenfunctions with $\Delta_{\mathbb{S}^1}$ in the (x_1, x_2), or (x, y), plane. (Is there a physical reason for using such a basis?) That means the spherical harmonics in the basis, when restricted to $x_1^2 + x_2^2 + x_3^2 = 1$, are also circular harmonics with respect to the x_1 and x_2 basis. Thus instead of $x_3^2 - x_1^2$ one uses $3x_3^2 - 1$, which is labeled as z^2.

References

[Bo] David Borthwick, *Introduction to Partial Differential Equations*. Springer, 2016.

[Ta] Michael E. Taylor, *Introduction to Analysis in Several Variables*, AMS Sally Series of Pure and Applied Undergraduate Texts 46, 2020. Preprint available online at https://mtaylor.web.unc.edu/wp-content/uploads/sites/16915/2018/04/analmv.pdf.