Differentiating Spherical Harmonics

Guohao Dou

January 11, 2020

1 Definition and Notation

The definition of spherical harmonics(SH) as discussed here, complex or real, is mostly in accordance with the SciPy definition[1] (without the Condon–Shortley phase). Here ν is the zenith angle and φ the azimuth angle.

For $l = 0, 1, 2, 3...$ and $m = -l, ..., -2, -1, 0, 1, 2, \dots l$

$$Y_l^m(\nu, \varphi) := \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\nu) e^{jm\varphi}, \quad \nu \in (0, \pi), \varphi \in (0, 2\pi)$$

where P_l^m is the associated normalized Legendre function of the first kind. They satisfy the parity condition,

$$P_l^{-m} = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m$$

This parity condition of Legendre functions is one of the main motivations for the funky $\frac{(l-m)!}{(l+m)!}$ term in SH. Note that for $m > 0$,

$$\begin{aligned}
Y_l^{-m}(\nu, \varphi) &= \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}} P_l^{-m}(\cos\nu) e^{-jm\varphi} \\
&= (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}} \frac{(l-m)!}{(l+m)!} P_l^m(\cos\nu) e^{-jm\varphi} \\
&= (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\nu) e^{-jm\varphi} \\
&= (-1)^m (Y_l^m)^*(\nu, \varphi)
\end{aligned}$$

where the star $*$ indicates complex conjugate. In short,

$$Y_l^{-m} = (-1)^m (Y_l^m)^*$$

There're many alternative definitions of SH out there. But almost all of them will make sure that this parity condition holds. Good to keep in mind!

Also, we should remind ourselves that all these mind-boggling normalizers have but one purpose of existence: to make

$$\langle Y_l^m, Y_k^n \rangle := \int_{S^2} (Y_l^m)^* Y_k^n dv = \delta_n^m \delta_k^l$$

that is, they form an orthonormal basis. Note that without these normalizers they are still orthogonal to each other and can still be useful. Even though 99% of pain in learning about SHs comes from the normalizing factors, orthonormality is not extremely meaningful except for the Copenhagen interpretation of quantum mechanics where $\Psi^*\Psi$ is viewed as probability density functions and should be integrated to 1 by definition.

The first few of P_l^m are defined as:

$$P_0^0(\cos\nu) = 1$$

$$P_1^{-1}(\cos\nu) = \frac{1}{2}\sin\nu, P_1^0(\cos\nu) = \cos\nu, P_1^1(\cos\nu) = -\sin\nu$$

$$P_2^0(\cos\nu) = \frac{1}{2}(3\cos^2\nu - 1), P_2^1(\cos\nu) = -3\cos\nu\sin\nu, P_2^2(\cos\nu) = 3\sin^2\nu$$

$$...(2l+1) \text{ different } P_l^m \text{ at degree } l...$$

In consequence, the first few SHs are defined as following:

$$Y_0^0(\nu,\varphi) := \sqrt{\frac{1}{4\pi}}$$

$$Y_1^{-1}(\nu,\varphi) := \sqrt{\frac{3}{8\pi}}\sin(\nu)e^{-i\varphi}, \quad Y_1^0(\nu,\varphi) := \sqrt{\frac{3}{4\pi}}\cos\nu, \quad Y_1^1(\nu,\varphi) := -\sqrt{\frac{3}{8\pi}}\sin(\nu)e^{i\varphi}$$

A few lines of code show that SciPy is happy about the way SHs are defined.

```
In [2]: from scipy.special import sph_harm
        import numpy as np


        def sh(l, m, zenith, azimuth):
            return sph_harm(m, l, azimuth, zenith)
```

```
In [7]: azimuth = np.pi / 4
        zenith = np.pi / 6
        y11 = sh(1, 1, zenith, azimuth)
        y11

Out[7]: (-0.12215062797572998-0.12215062797572995j)
```

```
In [10]: my_y11 = -np.sqrt(3 / (8 * np.pi)) * np.sin(zenith) * np.exp(1j * azimuth)
         my_y11

Out[10]: (-0.12215062797572998-0.12215062797572995j)
```

```
In [11]: y1n1 = sh(1, -1, zenith, azimuth)
         y1n1

Out[11]: (0.12215062797572998-0.12215062797572995j)
```

```
In [12]: my_y1n1 = np.sqrt(3 / (8 * np.pi)) * np.sin(zenith) * np.exp(-1j * azimuth)
         my_y1n1

Out[12]: (0.12215062797572998-0.12215062797572995j)
```

There are indeed a few cases where the real spherical harmonics (RSH) can be useful. Denote them as $\mathcal{Y}_l^m$ and they are defined as:

$$\mathcal{Y}_l^m = \begin{cases} \frac{1}{\sqrt{2}}(Y_l^m + (-1)^m Y_l^{-m}) = \sqrt{2}\,\mathrm{Re}[Y_l^m] & m > 0 \\ Y_l^0 & m = 0 \\ \frac{1}{j\sqrt{2}}(Y_l^{-m} - (-1)^m Y_l^m) = \sqrt{2}\,\mathrm{Im}[Y_l^{-m}] & m < 0 \end{cases}$$

As usual, the mysterious factor $\frac{1}{\sqrt{2}}$ comes from the mysterious need for orthonormality. Note that

$$\begin{aligned} &\langle \frac{1}{\sqrt{2}}(Y_l^m + (-1)^m Y_l^{-m}), \frac{1}{\sqrt{2}}(Y_l^m + (-1)^m Y_l^{-m})\rangle \\ =&\frac{1}{2}[\langle Y_l^m, Y_l^m\rangle + \langle Y_l^{-m}, Y_l^{-m}\rangle \\ &+ (-1)^m\langle Y_l^m, Y_l^{-m}\rangle + (-1)^m\langle Y_l^{-m}, Y_l^m\rangle] \\ =&\frac{1}{2}(1+1) = 1 \end{aligned}$$

2 Partial Derivative

If we think carefully about it, we'll see that Y_l^m are complex-valued functions defined on S^2. Taking partial derivative of such a function may not be the most mathematically rigorous thing to do, but let's try it anyway.

2.1 What Mathematica Tells Me

Fact 1. *The partial derivative of Y_l^m, $\frac{\partial Y_l^m}{\partial \nu}$, $\frac{\partial Y_l^m}{\partial \varphi}$, can be efficiently evaluated using the following recurrence formula:*

$$\begin{aligned} \frac{\partial Y_l^m}{\partial \nu} &= m\cot\nu Y_l^m + \sqrt{(l+m+1)(l-m)}e^{-i\varphi}Y_l^{m+1} \\ \frac{\partial Y_l^m}{\partial \varphi} &= jmY_l^m \end{aligned}$$

Example 1. The formula above looks almost too good to be true and I can see you have trust issues. Let's try it out on

$$Y_2^1(\nu,\varphi) = -\sqrt{\frac{15}{8\pi}}\cos\nu\sin\nu e^{j\varphi}$$

$$\begin{aligned} LHS &:= \frac{\partial Y_2^1}{\partial \nu} = \sqrt{\frac{15}{8\pi}}(\sin^2\nu - \cos^2\nu)e^{j\varphi} \\ RHS &:= \cot\nu Y_2^1 + \sqrt{4}e^{-j\varphi}Y_2^2 \\ &= -\sqrt{\frac{15}{8\pi}}\cos^2\nu e^{j\varphi} + \sqrt{4}e^{-j\varphi}\sqrt{\frac{15}{32\pi}}\sin^2\nu e^{j2\varphi} \\ &= \sqrt{\frac{15}{8\pi}}(\sin^2\nu - \cos^2\nu)e^{j\varphi} = LHS \end{aligned}$$

And it works out just fine. Let's try another,

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\nu$$

$$\begin{aligned}
LHS &:= \frac{\partial Y_1^0}{\partial \nu} = -\sqrt{\frac{3}{4\pi}} \sin\nu \\
RHS &:= \sqrt{2\cdot 1} e^{-j\varphi} Y_1^1 \\
&= \sqrt{2} e^{-j\varphi} \left(-\sqrt{\frac{3}{8\pi}} \sin\nu e^{j\varphi} \right) \\
&= -\sqrt{\frac{3}{4\pi}} \sin\nu = LHS
\end{aligned}$$

Remark 1. Note that the formula will seemingly break when it's applied on Y_l^l, since Y_l^{l+1} doesn't make any sense. In that case, note that the $\sqrt{(l+m+1)(l-m)}$ term will be zero and take care of this rogue case. If it still feels unsettling, simply make a special case:

$$\frac{\partial Y_l^l}{\partial \nu} = l \cot\nu Y_l^l$$

Try it out on

$$Y_2^2 = \sqrt{\frac{15}{32\pi}} \sin^2\nu e^{j2\varphi}$$

$$\frac{\partial Y_2^2}{\partial \nu} = \sqrt{\frac{15}{32\pi}} 2 \sin\nu \cos\nu e^{j2\varphi} = 2 \cot\nu Y_2^2$$

works like a charm.

2.2 Polar Singularity

We should note that the formula listed above will fail miserably when $\nu = 0$ or $\nu = \pi$. Even though SHs with $m \neq 0$ will be zero at poles, the product, $\cot\nu Y_l^m$ will not necessarily go to zero. A quick counterexample would be Y_2^1:

$$\cot\nu Y_2^1 = -\sqrt{\frac{15}{8\pi}} \cos^2\nu e^{j\varphi}$$

and this obviously looks very non-zero at poles.

This issue requires a serious solution and cannot be simply swept under the rock. We should make use of the following recurrence formula for $m \geq 1$:

$$\frac{P_l^m}{\sin\nu} = -\frac{1}{2m} \left[(l+m)(l+m-1) P_{l-1}^{m-1} + P_{l-1}^{m+1} \right]$$

where the second term is defined as zero if $m+1 > l-1$

It is a tedious exercise to rewrite it in terms of SH.

$$\begin{aligned}
m\cot\nu Y_l^m = &-\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l+m)(l+m-1)}Y_{l-1}^{m-1}e^{j\varphi} \\
&-\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l-m)(l-m-1)}Y_{l-1}^{m+1}e^{-j\varphi}
\end{aligned}$$

which somehow exhibits a satisfying symmetry.

Even if the formula only makes sense for $m \geq 1$, we could use the parity property to get what we want. First notice that when $m = 0$, the term simply vanishes like it has never existed. Then for the case $-m \leq -1$ ($m \geq 1$),

$$\begin{aligned}
-m\cot\nu Y_l^{-m} &= -m\cot\nu(-1)^m(Y_l^m)^* \\
&= (-1)^{m+1}(m\cot\nu Y_l^m)^* \\
&= -\frac{(-1)^{m+1}}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l+m)(l+m-1)}(Y_{l-1}^{m-1})^*e^{-j\varphi} \\
&\quad -\frac{(-1)^{m+1}}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l-m)(l-m-1)}(Y_{l-1}^{m+1})^*e^{j\varphi} \\
&= -\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l+m)(l+m-1)}Y_{l-1}^{1-m}e^{-j\varphi} \\
&\quad -\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l-m)(l-m-1)}Y_{l-1}^{-m-1}e^{j\varphi}
\end{aligned}$$

Stop for a brief moment and observe that if you let $n = -m \leq 1$, the equation above becomes

$$\begin{aligned}
n\cot\nu Y_l^n = &-\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l+n)(l+n-1)}Y_{l-1}^{n-1}e^{j\varphi} \\
&-\frac{1}{2}\sqrt{\frac{2l+1}{2l-1}}\cos\nu\sqrt{(l-n)(l-n-1)}Y_{l-1}^{n+1}e^{-j\varphi}
\end{aligned}$$

which is exactly the same formula as $m \geq 1$. That means when implementing them in software there's no need to code them up again. However, use some caution when checking whether the order $m-1$ and $m+1$ exceed the acceptable range.

We have reasons to believe that this new formula will not only remove polar singularity but be more numerically stable as well, since we no longer have to divide by $\sin\nu$.

References

[1] Eric Jones, Travis Oliphant, Pearu Peterson, et al. SciPy: Open source scientific tools for Python, 2001–. [Online; accessed Oct. 17 2019].