LEGENDRE POLYNOMIALS - ORTHOGONALITY

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.6.

In another post, we found that the Legendre polynomials could be written as an explicit sum as follows

$$P_n(x) = \sum_{k=0}^{[n/2]} \frac{(2n-2k)!}{2^n (n-k)!k!(n-2k)!} (-1)^k x^{n-2k} \tag{1}$$

This can be written as a derivative if we observe that if $k \le [n/2]$

$$\frac{d^n}{dx^n} x^{2n-2k} = \frac{(2n-2k)!}{(n-2k)!} x^{n-2k} \tag{2}$$

Note that if $k > [n/2]$, the n^{th} derivative of x^{2n-2k} is zero, since after $[n/2]$ derivatives, the term x^{2n-2k} is reduced to a constant. We can use this fact to rewrite the sum above as

$$P_n(x) = \sum_{k=0}^{[n/2]} \frac{(-1)^k}{2^n (n-k)!k!} \frac{d^n}{dx^n} x^{2n-2k} \tag{3}$$

$$= \sum_{k=0}^{n} \frac{(-1)^k}{2^n (n-k)!k!} \frac{d^n}{dx^n} x^{2n-2k} \tag{4}$$

$$= \frac{1}{2^n n!} \sum_{k=0}^{n} \frac{(-1)^k n!}{(n-k)!k!} \frac{d^n}{dx^n} x^{2n-2k} \tag{5}$$

$$= \frac{1}{2^n n!} \frac{d^n}{dx^n} \sum_{k=0}^{n} \frac{(-1)^k n!}{(n-k)!k!} x^{2n-2k} \tag{6}$$

The sum in the last line is the binomial expansion of $(x^2-1)^n$ (since the factorials within the sum form the binomial coefficient $\left(\begin{array}{c} n \\ k \end{array}\right)$), so we can write this as

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2-1)^n \tag{7}$$

This is known as the Rodrigues formula for Legendre polynomials. Although it's not all that convenient for calculating the polynomials themselves, it can be used to prove various properties about them. One of the most important theorems is that the polyomials are orthogonal. This means that if $n \neq m$, we have

$$\int_{-1}^{1} P_m(x) P_n(x) dx = 0 \tag{8}$$

This property turns out to be of vital importance in quantum mechanics, where the polynomials form the basis of the associated Legendre functions, which in turn form part of the solution of the three-dimensional Schrödinger equation. We'll run through the proof here.

Using the Rodrigues formula, we have

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \frac{1}{2^{m+n} m! n!} \int_{-1}^{1} \frac{d^m}{dx^m} (x^2-1)^m \frac{d^n}{dx^n} (x^2-1)^n dx \tag{9}$$

Before doing the integration, we note that all derivatives of the function $(x^2-1)^m$ up to the $(m-1)$th derivative have x^2-1 as a factor (we can see this by applying the chain rule), and are therefore zero at $x = \pm 1$. Now assume that $m < n$ for the purposes of being definite (it won't matter if $m > n$ since we can just swap the two indexes throughout the argument).

If we integrate 9 by parts we get

$$\int_{-1}^{1} \frac{d^m}{dx^m} (x^2-1)^m \frac{d^n}{dx^n} (x^2-1)^n dx = \frac{d^{n-1}}{dx^{n-1}} (x^2-1)^n \frac{d^m}{dx^m} (x^2-1)^m \Big|_{-1}^{1} - \tag{10}$$

$$\int_{-1}^{1} \frac{d^{m+1}}{dx^{m+1}} (x^2-1)^m \frac{d^{n-1}}{dx^{n-1}} (x^2-1)^n dx \tag{11}$$

Because of the condition just stated, the boundary term at the start is zero, so we can continue by integrating the remaining integral by parts, throwing away the boundary term until we have done n integrations. At this point we will have

$$\int_{-1}^{1} P_m(x) P_n(x) dx = \frac{1}{2^{m+n} m! n!} (-1)^n \int_{-1}^{1} (x^2-1)^n \frac{d^{m+n}}{dx^{m+n}} (x^2-1)^m dx \tag{12}$$

Since $m<n$, the derivative inside the integral is zero, since the largest power of x in $(x^2-1)^m$ is x^{2m} and $2m<m+n$. Therefore, the overall integral is zero, and we have shown that the Legendre polynomials are orthogonal (that is, 8 is true).

What if $n=m$? In that case, the integration by parts technique won't work, since we can't count on the final integral being zero. However, after n integrations by parts, we get to the formula

$$\int_{-1}^{1} P_n(x)P_n(x)dx = \frac{(-1)^n}{(n!)^2 2^{2n}}\int_{-1}^{1}(x^2-1)^n \frac{d^{2n}}{dx^{2n}}(x^2-1)^n dx \tag{13}$$

The deriviatve inside the integral will kill off all terms within $(x^2-1)^n$ except for the highest power of x^{2n} and the derivative of that is

$$\begin{aligned} \frac{d^{2n}}{dx^{2n}}(x^2-1)^n &= \frac{d^{2n}}{dx^{2n}}x^{2n} && (14)\\ &= (2n)! && (15)\end{aligned}$$

We can therefore write

$$\int_{-1}^{1} P_n(x)P_n(x)dx = \frac{(-1)^n(2n)!}{(n!)^2 2^{2n}}\int_{-1}^{1}(x^2-1)^n dx \tag{16}$$

The final integral can be done by using a trigonometric substitution (e.g. $x=\sin\theta$ so $x^2-1=-\cos\theta$ and $dx=\cos\theta d\theta$). This still requires the integration of a high power of $\cos\theta$ so we can take the easy way out and use mathematical software such as Maple or Mathematica to do the integral directly. In that case we find

$$\int_{-1}^{1}(x^2-1)^n dx = \frac{(-1)^n\Gamma(n+1)\sqrt{\pi}}{\Gamma(n+3/2)} \tag{17}$$

The gamma function $\Gamma(x)$ is a generalization of the factorial function and has a number of convenient properties we can use to simplify this (we'll leave the derivation of these properties to another post). In particular, we have

$$\begin{aligned} \Gamma(n+1) &= n! && (18)\\ \Gamma(z)\Gamma(z+1/2) &= 2^{1-2z}\sqrt{\pi}\Gamma(2z) && (19)\end{aligned}$$

The second of these formulas (known as the duplication formula) can be used to show that

$$\Gamma(n+3/2)=\Gamma((n+1)+1/2)=\frac{\sqrt{\pi}(2n+1)!}{2^{1+2n}n!} \tag{20}$$

so plugging this into 17 we find that

$$\int_{-1}^{1}(x^2-1)^n dx = (-1)^n\frac{(n!)^2 2^{1+2n}}{(2n+1)!} \tag{21}$$

so plugging this back into 16 we get finally

$$\begin{aligned}\int_{-1}^{1}P_n(x)P_n(x)dx &= \frac{1}{(n!)^2 2^{2n}}(2n)!(-1)^{2n}\frac{(n!)^2 2^{1+2n}}{(2n+1)!} &(22)\\ &= \frac{2}{2n+1} &(23)\end{aligned}$$

We can combine the results on integration of the Legendre polynomials to get the overall orthogonality condition:

$$\int_{-1}^{1}P_n(x)P_m(x)dx=\frac{2}{2n+1}\delta_{nm} \tag{24}$$