ASSOCIATED LEGENDRE FUNCTIONS - ORTHOGONALITY

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We have found in another post the associated Legendre functions which are solutions of the general Legendre equation

$$\frac{d}{dx}\left((1-x^2)\frac{dP}{dx}\right)+\left[l(l+1)-\frac{m^2}{1-x^2}\right]P=0 \tag{1}$$

In terms of the Legendre polynomials, the associated Legendre functions can be written as

$$P_l^m(x)=(1-x^2)^{m/2}\frac{d^mP_l(x)}{dx^m} \tag{2}$$

Although we can continue from this point and write the functions as explicit sums, in this post we want to prove something else: that the associated Legendre functions are a set of orthogonal functions. This property is of importance in quantum mechanics, among other places in physics, so we need to establish this foundation of the theory.

To proceed, we can use the Rodrigues formula for the Legendre polynomials:

$$P_l(x)=\frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l \tag{3}$$

Inserting this into 2, we get

$$P_l^m(x)=\frac{1}{2^l l!}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \tag{4}$$

We can make the notation a bit simpler by defining

$$X(x)\equiv(x^2-1) \tag{5}$$

We can then rewrite 4 as

$$P_l^m(x)=\frac{1}{2^l l!}(-X)^{m/2}\frac{d^{l+m}X^l}{dx^{l+m}} \tag{6}$$

At this point, we can pause to notice that this definition allows us to let m range over negative values as well as positive, so we can use this as a definition of the associated Legendre functions for $-l\le m\le l$.

Now to the orthogonality condition. Since the functions are defined over the range $-1 \leq x \leq 1$ we need to evaluate the integral $\int_{-1}^{1} P_p^m P_q^m dx$ for some values p and q. Note that we are restricting m to be the same in both functions. First, we'll consider the case $p < q$ which covers all cases where the lower indexes are unequal. Using 6, we can write

$$\int_{-1}^{1} P_p^m P_q^m dx = \frac{(-1)^m}{2^{p+q} p! q!} \int_{-1}^{1} X^m \frac{d^{p+m} X^p}{dx^{p+m}} \frac{d^{q+m} X^q}{dx^{q+m}} dx \tag{7}$$

Now we can use integration by parts to write

$$\int_{-1}^{1} P_p^m P_q^m dx = \frac{(-1)^m}{2^{p+q} p! q!} \left[\frac{d^{q+m-1} X^q}{dx^{q+m-1}} X^m \frac{d^{p+m} X^p}{dx^{p+m}} \Big|_{-1}^{1} - \int_{-1}^{1} \frac{d^{q+m-1} X^q}{dx^{q+m-1}} \frac{d}{dx} \left(X^m \frac{d^{p+m} X^p}{dx^{p+m}} \right) dx \right] \tag{8}$$

The integrated term will be zero, since $X = 0$ at both endpoints. Thus

$$\int_{-1}^{1} P_p^m P_q^m dx = \frac{(-1)^m (-1)}{2^{p+q} p! q!} \int_{-1}^{1} \frac{d^{q+m-1} X^q}{dx^{q+m-1}} \frac{d}{dx} \left(X^m \frac{d^{p+m} X^p}{dx^{p+m}} \right) dx \tag{9}$$

If we repeat the integration by parts, the integrated term is

$$\frac{d^{q+m-2} X^q}{dx^{q+m-2}} \frac{d}{dx} \left(X^m \frac{d^{p+m} X^p}{dx^{p+m}} \right) \tag{10}$$

The derivative in large parentheses in this term contains the factor X^{m-1} so (if $m > 1$) will again be zero at the endpoints. By the same reasoning, since the degree of the derivative of this term in parentheses increases by 1 on each integration, the j^{th} integration by parts will contain a factor of X^{m-j+1} provided $j \leq m$, and will therefore be zero.

If we integrate by parts beyond this point, the second derivative factor will no longer be zero at the endpoints. However, now the *first* derivative factor becomes $d^{q+m-j} X^q / dx^{q+m-j}$. Since $j > m$ at this stage, this derivative will now contain a factor of $X^{q-(q+m-j)} = X^{j-m}$ and will now be zero. (Actually, due to the product rule being applied successively as we calculate higher and higher derivatives, there will be a sum of terms, but the *lowest* power of X in any of these terms will be X^{j-m} so every term in the product rule sum will go to zero at the endpoints.)

That is, if we integrate by parts $q + m$ times, the integrated term will be zero at every stage, and we get for the final result:

$$\int_{-1}^{1} P_p^m P_q^m dx = \frac{(-1)^m (-1)^{q+m}}{2^{p+q} p! q!} \int_{-1}^{1} X^q \frac{d^{q+m}}{dx^{q+m}} \left(X^m \frac{d^{p+m}}{dx^{p+m}} X^p \right) dx \tag{11}$$

This might not look much better, but we can examine the integrand a bit more closely. The highest power of x in X^p is x^{2p}, so the highest power of x in $\frac{d^{p+m}}{dx^{p+m}}X^p$ is $x^{2p-p-m} = x^{p-m}$. Multiplying this by X^m, which has a highest power of x of x^{2m}, gives an overall leading term of $x^{p-m+2m} = x^{p+m}$. Now since we assumed $q > p$, taking the $(q+m)^{th}$ derivative of x^{p+m} (or any lower power) will always give zero, so we've shown that the integrand is always zero if $q \neq p$ (since p and q appeared symetrically in the original integral, the argument is exactly the same if we assume $q < p$). Thus the associated Legendre functions are orthogonal.

What if $p = q$? In that case, the derivative part of the integrand in 11 will be a constant, as we'll now see. We can work out $d^{p+m}(x^{2p})/dx^{p+m}$ first. Since each derivative brings down the exponent and then reduces the exponent by 1, we get

$$\frac{d^{p+m}}{dx^{p+m}}X^p = \frac{(2p)!}{(2p-(p+m))!}x^{2p-(p+m)} + \ldots \tag{12}$$

$$= \frac{(2p)!}{(p-m)!}x^{p-m} + \ldots \tag{13}$$

Similarly, we get

$$\frac{(2p)!}{(p-m)!}\frac{d^{p+m}}{dx^{p+m}}(X^m x^{p-m}) = \frac{(2p)!}{(p-m)!}\frac{d^{p+m}}{dx^{p+m}}(x^{2m}x^{p-m} + \ldots) \tag{14}$$

$$= \frac{(2p)!}{(p-m)!}\frac{d^{p+m}}{dx^{p+m}}(x^{p+m} + \ldots) \tag{15}$$

$$= \frac{(2p)!}{(p-m)!}(p+m)! \tag{16}$$

Note that the final derivative kills off all lower powers of x so we need consider only the leading term. Substituting all this back into 11 with $p = q$ we get

$$\int_{-1}^{1}(P_p^m)^2 dx = \frac{(-1)^{p+2m}}{2^{2p}(p!)^2}\frac{(2p)!}{(p-m)!}(p+m)!\int_{-1}^{1}X^p dx \tag{17}$$

$$= \frac{(-1)^{p+2m}}{2^{2p}(p!)^2}\frac{(2p)!}{(p-m)!}(p+m)!\int_{-1}^{1}(x^2-1)^p dx \tag{18}$$

The integral is the same one we ran into when calculating the orthogonality of the Legendre polynomials, so we can just quote the result here:

$$\int_{-1}^{1}(x^2-1)^p dx = (-1)^p \frac{(p!)^2 2^{1+2p}}{(2p+1)!} \tag{19}$$

The final result is then

$$\int_{-1}^{1}(P_p^m)^2 dx = \frac{2}{2p+1}\frac{(p+m)!}{(p-m)!} \tag{20}$$

or, combining the orthogonality results:

$$\int_{-1}^{1}P_p^m P_q^m dx = \frac{2}{2p+1}\frac{(p+m)!}{(p-m)!}\delta_{pq} \tag{21}$$

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