Spherical Harmonics

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Created: March 2, 1999

This came up in verifying some potential equations arising from fast solution of the n–body problem.

Associated Lagrange functions are $P_n^m(u)$ for $n \geq 0$ and $-n \leq m \leq n$. Index n is called the degree, index m is called the order. They are defined by the following.

- Zero order:
$$P_n^0(u) = \frac{(-1)^n}{2^n n!} \frac{d^n}{du^n}(1-u^2)^n =: P_n(u)$$
- Positive order:
$$P_n^m(u) = (1-u^2)^{m/2} \frac{d^m}{du^m} P_n(u), \ m > 0$$
- Negative order:
$$P_n^{-m}(u) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(u), \ m > 0$$

To compute the nonnegative order terms (in a memoized way), use the following scheme. The negative order terms are then easily constructed using the definition above. First note that

$$P_n^n(u) = \frac{(1-u^2)^{n/2}}{2^n n!} \frac{d^{2n}}{du^{2n}}(u^2-1)^n = \frac{(2n)!(1-u^2)^{n/2}}{2^n n!}. \tag{1}$$

for $n \geq 0$. These are the initial conditions. The recursive formulas are

$$P_n^m(u) = \frac{(2n-1)uP_{n-1}^m(u) - (n+m-1)P_{n-2}^m(u)}{n-m} \tag{2}$$

for $n \geq 2$, and

$$P_n^m(u) = \frac{(1-u^2)^{1/2}}{2mu} \left(P_n^{m+1}(u) + (n+m)(n-m+1)P_n^{m-1}(u) \right) \tag{3}$$

for $m \geq 1$. Let `P(n,m)` represent the value of $P_n^m(u)$. The pseudocode to evaluate all of $P_N^m(u)$ for specified N and u is

```
P(0,0) = 1;
P(1,0) = u;
P(1,1) = sqrt(1-u*u);
for (n = 2; n <= N; n++)
{
    evaluate P(n,n) using equation (1);
    for (m = 0; m <= n-2; m++)
        evaluate P(n,m) using equation (2);
    evaluate P(n,n-1) using equation (3);
}
```

The following table shows values for $P_n^m(u)$ for $n \le 3$.

$$
\begin{array}{llll}
 & & & P_3^3 = 15(1-u^2)^{3/2} \\
 & & P_2^2 = 3(1-u^2) & P_3^2 = 15u(1-u^2) \\
 & P_1^1 = (1-u^2)^{1/2} & P_2^1 = 3u(1-u^2)^{1/2} & P_3^1 = \frac{3}{2}(5u^2-1)(1-u^2)^{1/2} \\
P_0^0 = 1 & P_1^0 = u & P_2^0 = \frac{1}{2}(3u^2-1) & P_3^0 = \frac{1}{2}u(5u^2-3) \\
 & P_1^{-1} = -\frac{1}{2}(1-u^2)^{1/2} & P_2^{-1} = -\frac{1}{2}u(1-u^2)^{1/2} & P_3^{-1} = -\frac{1}{8}(5u^2-1)(1-u^2)^{1/2} \\
 & & P_2^{-2} = \frac{1}{8}(1-u^2) & P_3^{-2} = \frac{1}{8}u(1-u^2) \\
 & & & P_3^{-3} = -\frac{1}{48}(1-u^2)^{3/2}
\end{array}
$$

The derivatives of the associated Legendre functions can be computed using the following formula:

$$\frac{dP_n^m}{du} = \frac{muP_n^m - (n+m)(n-m+1)\sqrt{1-u^2}P_n^{m-1}}{1-u^2}. \tag{4}$$

When $m = 0$, the formula involves functions of order -1. If you want to compute derivatives only using functions of nonnegative order, use the definition for the negative order functions:

$$\frac{dP_n}{du} = \frac{-n(n+1)P_n^{-1}}{\sqrt{1-u^2}} = \frac{P_n^1}{\sqrt{1-u^2}}. \tag{5}$$

Let `DP(n,m)` represent the value of $dP_n^m(u)/du$. The pseudocode to evaluate all of $dP_N^m(u)/du$ for specified N and u is as follows. First compute all of $P_n^m(u)$ for $n \le N$; then use

```
DP(0,0) = 0;
for (n = 1; n <= N; n++) {
    evaluate DP(n,0) using equation (5)
    for (m = 1; m <= n; m++)
        evaluate DP(n,m) using equation (4)
}
```

For derivatives of negative order functions, just use the definition relating the negative order functions to the positive order functions.

The following table shows values for $dP_n^m(u)/du$ for $n \le 3$.

			$DP_3^3 = -45(1-u^2)^{1/2}$
		$DP_2^2 = -6u$	$DP_3^2 = 15(1-3u^2)$
	$DP_1^1 = \frac{-u}{\sqrt{1-u^2}}$	$DP_2^1 = \frac{3(1-2u^2)}{\sqrt{1-u^2}}$	$DP_3^1 = \frac{3}{2}\frac{u(11-15u^2)}{\sqrt{1-u^2}}$
$DP_0^0 = 0$	$DP_1^0 = 1$	$DP_2^0 = 3u$	$DP_3^0 = \frac{3}{2}(5u^2-1)$
	$DP_1^{-1} = \frac{1}{2}\frac{u}{\sqrt{1-u^2}}$	$DP_2^{-1} = -\frac{1}{2}\frac{(1-2u^2)}{\sqrt{1-u^2}}$	$DP_3^{-1} = -\frac{1}{8}\frac{u(11-15u^2)}{\sqrt{1-u^2}}$
		$DP_2^{-2} = -\frac{1}{4}u$	$DP_3^{-2} = \frac{1}{8}(1-3u^2)$
			$DP_3^{-3} = \frac{1}{16}u(1-u^2)^{1/2}$

Note that the functions $dP_n^{\pm 1}/du$ are unbounded at $u = \pm 1$, so you may have numerical problems to deal with at those points.

The spherical harmonic functions are defined by

$$Y_n^m(\theta,\phi) = \sqrt{\frac{(n-|m|)!}{(n+|m|)!}}P_n^m(\cos\theta)\exp(im\phi)$$

for $n \ge 0$ and $-n \le m \le n$. Spherical coordinates are $x = r\cos\phi\sin\theta$, $y = r\sin\phi\sin\theta$, and $z = r\cos\theta$. The potential function $\Phi(r,\theta,\phi)$ which satisfies Laplaces equation

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\Phi\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\phi^2} = 0$$

is

$$\Phi = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(L_n^m r^n + M_n^m r^{-(n+1)}\right)Y_n^m(\theta,\phi).$$

The L constants are 0 for the multipole expansion; the M constants are 0 for the local expansion.

To compute the gradient of Φ, in spherical coordinates,

$$\nabla\Phi = \frac{\partial\Phi}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial\Phi}{\partial\theta}\vec{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial\Phi}{\partial\phi}\vec{e}_\phi$$

where $\vec{e}_r = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$, $\vec{e}_\theta = (\cos\phi\cos\theta, \sin\phi\cos\theta, -\sin\phi)$, and $\vec{e}_\phi = (-\sin\phi, \cos\phi, 0)$. The r derivative is

$$\begin{aligned}\frac{\partial\Phi}{\partial r} &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(nL_n^m r^{n-1} - (n+1)M_n^m r^{-(n+2)}\right)Y_n^m(\theta,\phi)\\ &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(nL_n^m r^{n-1} - (n+1)M_n^m r^{-(n+2)}\right)\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}P_n^m(\cos\theta)\exp(im\phi).\end{aligned}$$

You need to compute the functions $P_n^m(\cos\theta)$ using the recursions given earlier, where the evaluation point is $u = \cos\theta$. The ϕ derivative is

$$\begin{aligned}\frac{\partial\Phi}{\partial\phi} &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(L_n^m r^n + M_n^m r^{-(n+1)}\right)\frac{\partial Y_n^m(\theta,\phi)}{\partial\phi}\\ &= \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left(L_n^m r^n + M_n^m r^{-(n+1)}\right)im\sqrt{\frac{(n-|m|)!}{(n+|m|)!}}P_n^m(\cos\theta)\exp(im\phi).\end{aligned}$$

Again, you need only compute the functions $P_n^m(\cos\theta)$ using the recursions with $u = \cos\theta$. The θ derivative is

$$
\begin{aligned}
\frac{\partial \Phi}{\partial \theta} &= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(L_n^m r^n + M_n^m r^{-(n+1)} \right) \frac{\partial Y_n^m(\theta,\phi)}{\partial \theta} \\
&= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left(L_n^m r^n + M_n^m r^{-(n+1)} \right) \sqrt{\frac{(n-|m|)!}{(n+|m|)!}} \frac{dP_n^m(\cos\theta)}{du} (-\sin\theta) \exp(im\phi).
\end{aligned}
$$

Now you need to compute the functions dP_n^m/du using the recursion formula given earlier for the derivatives of associated Legendre functions.