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On the Computation of Derivatives of Legendre Functions

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Abstract. Analysis and evaluation of spherical harmonics are important for Earth sciences and potential theory. Depending on the functional of the harmonic series, Legendre functions, their derivatives or their integrals must be computed numerically which in general is based on recurrence relations. Numerical stability and optimization of such recurrence relations become more and more important with increasing degree and order. In this paper, a simple relation is recovered to obtain first and higher order derivatives of Legendre functions. The relation is shown to be numerical stable, it does not cause a singularity at the poles, and can be applied recursively to obtain second and higher order derivatives. Moreover, it can be applied to compute integrals over derivatives of Legendre functions, quantities required if, for example, mean values of deflections of the vertical are to be analyzed or evaluated. A sample FORTRAN code is given and a few additional formulas used to verify the code and to investigate round-off errors for degree and order up to 360.

1 Introduction

An important tool to represent phenomena on the sphere are spherical harmonic series

$$Y(\lambda,\theta) = \sum_{n=0}^{N} Y_n(\lambda,\theta),$$

where

$$Y_n(\lambda,\theta) = \sum_{m=0}^{n} (C_{nm}\cos m\lambda + S_{nm}\sin m\lambda) P_{nm}(\cos\theta)$$

with longitude λ, colatitude θ, the harmonic coefficients C_{nm} and S_{nm} of degree n and order m, and the associated Legendre functions of the first kind P_{nm} .

The evaluation of such series often requires to perform derivatives with respect to colatitude θ, e.g., if the disturbing potential of the Earth gravity field is given in terms of spherical harmonics and north-south deflections of the vertical are to be derived. Simulation or analysis of gradiometer data requires to consider all second order derivatives of the Earth gravity field. Sometimes mean values of those quantities are to be computed or are given as "observed values" for a spherical harmonic analysis. In this case integrals of derivatives must be computed for a cell areas limited by meridians and parallels. In any way derivatives of Legendre functions or integrals over derivatives must be evaluated. The present paper recovers a simple recurrence relation that is convenient for numerical purposes. Other authors use more complicated relations and report about numerical problems at the poles ($\theta = 0$ or π). It will be shown that the algorithmic modifications suggested to overcome the polar singularity are unnecessary. Moreover, the simple relation can be applied recursively to obtain higher order derivatives of Legendre functions.

2 Basic Relations

For real $x = \cos\theta$ and integer degree n and order m the associated Legendre functions of the first kind are defined by [Kautzleben, 1965, p.30]:

$$P_{nm}(x) := (1 - x^2)^{m/2} \frac{d^m P_n(x)}{dx^m}$$

where $P_n(x)$ are Legendre polynomials of degree n. The definition above is consistent with Jahnke and Emde (1938) and Heiskanen and Moritz (1967) while Hobson (1931), Lense (1950), and Ryshik and Gradstein (1957) apply an additional factor $(-1)^m$ right hand that modifies the sign in those recurrence relations where the order m varies.

For the numerics of high degree and order, normalization of Legendre functions is essential because already at moderate degree and order overflows appear for the unnormalized functions due to the limited representation of floating point numbers. In spite of this we present the formulas of interest first for the unnormalized functions and give the normalized equations, necessary for a successful implementation working for higher degree and order in the appendix.

In the following, we denote the associated Legendre functions of the first kind simply as LF and we will use short-hand notation such as

$$P_{nm} := P_{nm}(\cos\theta).$$

For clarification the double index is separated by a comma, whenever one of the indices takes the form of an algebraic expression.

For completeness and later reference we give the basic recurrence relations for the LF. For *varying degree and order* we have [Kautzleben, p.34, Eq. 257a]

$$P_{nm} = (2n-1)\sin\theta P_{n-1,m-1} + P_{n-2,m}. \tag{1}$$

Note, $P_{nm} = 0$ for any $m > n$. This is obvious because the P_{nm} are defined by the m-th derivative of the Legendre polynomials P_n that are known to be homogeneous polynomials of degree n. Thus, the last term of Eq. (1) above vanishes for $m = n$ and $m = n-1$ and one obtains the special relations

$$P_{nn} = (2n-1)\sin\theta P_{n-1,n-1}, \tag{2}$$

$$P_{n,n-1} = (2n-1)\sin\theta P_{n-1,n-2}. \tag{3}$$

For *varying order* we have [ibid, p.34, Eq. 256a]

$$\begin{aligned} P_{n,m+2} &= (2m+1)\cot\theta P_{n,m+1} \\ &- (n-m)(n+m+1)P_{n,m}, \end{aligned} \tag{4}$$

for *varying degree* [ibid, p.34, Eq. 259a]

$$\begin{aligned} (2n+1)\cos\theta\, P_{nm} &= (n+m)P_{n-1,m} \\ &+ (n-m+1)P_{n+1,m}. \end{aligned} \tag{5}$$

3 Formulas for Derivatives

In contrast to the relations for the LF itself there is no equation relating only the derivatives of LF among each other. Derivatives of LF always appear with the LF itself. Following relations between the LF and their derivatives are given by Kautzleben [p.34f, Eq.s 260a and 264a]

$$\sin\theta\frac{dP_{nm}}{d\theta} = m\cos\theta\, P_{nm} - \sin\theta\, P_{n,m+1} \tag{6}$$

$$\sin\theta\frac{dP_{nm}}{d\theta} = n\cos\theta\, P_{nm} - (n+m)\, P_{n-1,m}. \tag{7}$$

The last one is sometimes represented after division by $\sin\theta$. Some authors obtain even more complicated equations, derived by differentiation of one of the recurrence relations for the LF itself. Tscherning (1976), for example, starts from Eq. (1) and performs first and second order derivatives. Wenzel (1985) derives a recurrence relation for the first order derivative by differentiation of Eq. (5). The problem with Eq. (6) and (7) and with the other relations just mentioned is that they can not be used at the poles. For $\theta = 0$ or $\theta = \pi$ the sin-function vanishes and - because $P_{nm}(\pm 1) \equiv 0$ for $m > 0$, both, Eq. (6) and (7) degenerate to trivial identities $0 = 0$. This failure was considered by Tscherning (1976) who suggested algorithmic modification to overcome the polar singularity. Sometimes, even a naive approach is applied by moving the point of computation a differential quantity away from the pole. It will be shown that this is completely unnecessary.

Given the LF, the derivatives can also be generated by [Kautzleben, p.35, Eq. 267]:

$$2\frac{dP_{nm}}{d\theta} = (n+m)(n-m+1)P_{n,m-1} - P_{n,m+1}, \tag{8}$$

a relation which is valid for $m > 0$ and easily derived by a combination of Eq.s (5), (6), and (7). For $m = 0$ we have the special relation

$$\frac{dP_{n0}}{d\theta} = -P_{n1} \tag{9}$$

following immediately from Eq. (6). It can also be derived from Eq. (8) when the equality [Kautzleben, p.31]

$$P_{n,-m} = (-1)^m \frac{(n-m)!}{(n+m)!} P_{nm}$$

valid for any m, is used to substitute $n(n+1)P_{n,-1}$ by $-P_{n,1}$. Because $P_{oo} = const$ we have

$$\frac{dP_{00}}{d\theta} = 0. \tag{10}$$

As already shown above, $P_{nm} = 0$ for any $m > n$. Thus for $m = n$ the last term of Eq. (8) vanishes and we obtain the relation

$$\frac{dP_{nn}}{d\theta} = nP_{n,n-1}. \tag{11}$$

4 Evaluation at the Poles

The relations (8), (9), (10) and (11) have remarkable advantages over those given by Eq. (6) and (7). First, there is no numerical problem at the poles ($\theta = 0$ or π). With $x = \cos\theta$ and $\theta = 0, \pi$ we have the special values

$$\begin{aligned} P_{nm}(\pm 1) &\equiv 0 \quad \text{for } m > 0, \\ P_{n0}(+1) &\equiv 1, \\ P_{n0}(-1) &\equiv (-1)^n. \end{aligned}$$

Thus, at the poles the only nonzero LFs are those for order $m = 0$. Considering Eq. (8) above the only nonzero first derivatives of the LF are those for order $m = 1$. Thus, at the poles the first order derivatives of harmonic series with respect to colatitude θ can be evaluated by

$$\frac{\partial}{\partial\theta}Y(\lambda,\theta) = \sum_{n=1}^{N} (C_{n1}\cos\lambda + S_{n1}\sin\lambda)\frac{dP_{n1}}{d\theta}.$$

The slopes at the poles are functions of longitude. In particular we have

$$\frac{dP_{n1}}{d\theta} = \frac{n(n+1)}{2} \quad \text{for } \theta = 0$$

and

$$\frac{dP_{n1}}{d\theta} = (-1)^n \frac{n(n+1)}{2} \quad \text{for } \theta = \pi.$$

Inserting this we obtain at the north pole ($\theta = 0$)

$$\frac{\partial}{\partial \theta} Y(\lambda) = \sum_{n=1}^{N} \frac{n(n+1)}{2} (C_{n1} cos\lambda + S_{n1} sin\lambda)$$

and at the south pole ($\theta = \pi$)

$$\frac{\partial}{\partial \theta} Y(\lambda) = \sum_{n=1}^{N} (-1)^n \frac{n(n+1)}{2} (C_{n1} cos\lambda + S_{n1} sin\lambda).$$

5 Second and Higher Order Derivatives

The second advantage is that the relation (8) above can be applied recursively in order to derive second and higher order derivatives. This is immediately clear because there is no sin- or cos-function such that there is no need to apply the product rule. Differentiating with respect to θ gives for $m > 0$

$$2\frac{d^2 P_{nm}}{d\theta^2} = (n+m)(n-m+1)\frac{dP_{n,m-1}}{d\theta} - \frac{dP_{n,m+1}}{d\theta} \qquad (12)$$

and for $n = 0$ and $m = n$ we obtain

$$\frac{d^2 P_{n0}}{d\theta^2} = -\frac{dP_{n1}}{d\theta} \qquad \frac{d^2 P_{nn}}{d\theta^2} = n\frac{dP_{n,n-1}}{d\theta}. \qquad (13)$$

The extension to higher order derivatives is trivial:

$$2\frac{d^k P_{nm}}{d\theta^2} = (n+m)(n-m+1)\frac{d^{k-1} P_{n,m-1}}{d\theta^{k-1}} - \frac{d^{k-1} P_{n,m+1}}{d\theta^{k-1}} \qquad (14)$$

Thus, one and the same algorithm can be used to derive first derivatives from the LF itself and second (and higher) order derivatives from the first (or lower order) derivatives.

Derivatives of order higher than two are seldom needed. Therefore, round-off error accumulation due to Eq. 14 is uncritical as long as this relation is not applied more than a few times. We conclude that the stability for getting low order derivatives by the Eq. (14) is governed by the stability of computing the LF itself.

6 Integrals of Derivatives

Integrals of Legendre functions are required whenever mean values of spherical harmonic series are to be evaluated or analyzed. Recurrence relations for the integrals were given by Paul (1978) and Gerstl (1978). Gerstl (1980) has shown how to apply the recurrence relations in order to obtain stable values of

$$IP_{nm} = \int_{\theta_1}^{\theta_2} P_{nm}(\cos\theta) \sin\theta d\theta$$

for any limits of integration.

In some cases it is even required to compute *integrals of derivatives* for the LF. Consider, for example, a spherical harmonic series representation of the Earth geopotential. In order to compute *mean values* for the north-south deflection of the verticals integrals of the first derivatives are required. A gradiometer mission observes second order derivatives of the disturbing potential and could - by means of data preprocessing - provide mean values for these second order derivatives. To analyze these mean values quantities of the form

$$ID^k P_{nm} = \int_{\theta_1}^{\theta_2} \frac{d^k P_{nm}(\cos\theta)}{d\theta^k} \sin\theta d\theta$$

are to be computed. An integration of Eq. (14) with limits θ_1 and θ_2 gives immediately following relation:

$$2ID^k P_{nm} = (n+m)(n-m+1) ID^{k-1} P_{n,m-1} - ID^{k-1} P_{n,m+1}. \qquad (15)$$

7 Verification

There are a few possibilities to verify the computation of derivatives of Legendre functions by Eq. (8).

1. For low degree and order the values of the derivatives can be compared with results obtains by using analytic formulas. We have done this up to degree and order 4 and found an maximum relative error of 0.5×10^{-16}. This agrees to the double precision that was used by the code and demonstrates that the recursion has been implemented right.

2. Next, it is possible to compare the results of Eq. (8) with the derivatives obtained by the alternative Eq.s (6) or (7). We performed this comparison for randomly selected arguments θ up to degree and order 360 and found a maximum relative discrepancy of about 0.5×10^{-11}. This indicates that the stability of Eq. (8) is not less than that of Eq. (6) or (7).

3. An additional test is possible by the differential equation for the Legendre Functions [Kautzleben, p.8]

$$\sin\theta\frac{d^2 P_{nm}}{d\theta^2} + \cos\theta\frac{dP_{nm}}{d\theta} + \left[\sin\theta n(n+1) - \frac{m^2}{\sin\theta}\right] P_{nm} = 0. \qquad (16)$$

Because this differential equation relates both, the first and second derivative with the LF itself it allows to investigate the round off-errors that accumulate by applying Eq. (8) twice. For this test, again performed for random θ and degree and order up to 360, we found a maximum relative error of the order of 0.5×10^{-9}.

8 Conclusion

A relation from Kautzleben (1967) has been recovered to obtain derivatives of Legendre functions. It is more simple than alternative formulae used so far. It is shown that the relation does not cause a singularity at the poles and that it can be applied recursively to compute higher order derivatives. In addition, it is demonstrated how to apply the relation to the computation of integrals over derivatives of Legendre functions. A FORTRAN code is provided with code verified by numerical tests with independent formulas.

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Appendix A Relations for normalized Legendre functions

Normalization of Legendre functions is also subject to different definition. Therefore we refer to the one given by Heiskanen/Moritz [1967, p.32]:

$$\bar{P}_{nm}(\cos\theta) := N_{n,m}P_{nm}(\cos\theta) \tag{A1}$$

with

$$N^2_{n,m} := (2-\delta_{0m})(2n+1)\frac{(n-m)!}{(n+m)!}. \tag{A2}$$

Multiplying Eq. (8) by $N_{n,m}$ we obtain

$$\begin{aligned} 2N_{n,m}\frac{dP_{nm}}{d\theta} &= (n+m)(n-m+1)N_{n,m}P_{n,m-1} \\ &\quad - N_{n,m}P_{n,m+1} \end{aligned}$$

or

$$\begin{aligned} 2\frac{d\bar{P}_{nm}}{d\theta} &= (n+m)(n-m+1)\frac{N_{n,m}}{N_{n,m-1}}\bar{P}_{n,m-1} \\ &\quad - \frac{N_{n,m}}{N_{n,m+1}}\bar{P}_{n,m+1}. \end{aligned} \tag{A3}$$

For the second right hand term we need the normalization factor for indices n and $m+1$

$$N^2_{n,m+1} = (2-\delta_{0,m+1})(2n+1)\frac{(n-m-1)!}{(n+m+1)!}$$

which can be rewritten as

$$N^2_{n,m+1} = N^2_{n,m}\frac{(2-\delta_{0,m+1})}{(2-\delta_{0,m})(n+m+1)(n-m)}.$$

Considering that $\delta_{0,m+1} = 0$ for any $m \geq 0$, it follows

$$\frac{N^2_{n,m}}{N^2_{n,m+1}} = (2-\delta_{0,m})\frac{(n+m+1)(n-m)}{2}. \tag{A4}$$

For the first term right hand of Eq. (A3) we get in just the same way

$$N^2_{n,m-1} = (2-\delta_{0,m-1})(2n+1)\frac{(n-m+1)!}{(n+m-1)!}$$

or

$$N^2_{n,m-1} = N^2_{n,m}\frac{(2-\delta_{0,m-1})(n+m)(n-m+1)}{(2-\delta_{0,m})}.$$

Because this factor does only appear for $m > 0$, the nominator simplifies to 2 and we finally have

$$\frac{N^2_{n,m}}{N^2_{n,m-1}} = \begin{cases} \frac{2}{n(n+1)} & \text{for } m = 1 \\ \frac{1}{(n+m)(n-m+1)} & \text{for } m > 1 \end{cases} \tag{A5}$$

If we insert Eq. (A4) and (A5) into Eq. (A3), we get for all $1 < m < n$

$$\begin{aligned} 2\frac{d\bar{P}_{nm}}{d\theta} &= \sqrt{(n+m)(n-m+1)}\bar{P}_{n,m-1} \\ &\quad - \sqrt{(n+m+1)(n-m)}\bar{P}_{n,m+1} \end{aligned} \tag{A6}$$

with the convenient property that the second square root factor is the same as the first square root factor with order m lowered by one. In addition we have the following special cases for $m = 0$

$$\frac{d\bar{P}_{00}}{d\theta} \equiv 0 \qquad \frac{d\bar{P}_{n0}}{d\theta} = -\sqrt{\frac{n(n+1)}{2}}\bar{P}_{n1}, \tag{A7}$$

for $m = 1$

$$\frac{d\bar{P}_{11}}{d\theta} = \bar{P}_{10}$$

$$2\frac{d\bar{P}_{n1}}{d\theta} = \sqrt{n(n+1)}\bar{P}_{n0} - \sqrt{(n-1)(n+2)}\bar{P}_{n2} \quad \text{(A8)}$$

and for $m = n > 1$

$$\frac{d\bar{P}_{nn}}{d\theta} = \sqrt{\frac{n}{2}}\bar{P}_{n,n-1}. \quad \text{(A9)}$$

The results have been used for a subroutine that generates the derivatives from the Legendre function and takes care of all special cases for both the unnormalized and the normalized functions.

Appendix B FORTRAN Code

The Eq.s (8) ... (11) and (A6) .. (A9) have been used to code a FORTRAN subroutine that performs first or higher order derivatives of the Legendre functions for both, the normalized and the unnormalized case. The code is available at the anonymous ftp ftp.dgfi.badw-muenchen.de at directory pub/altimetry or by email to bosch@dgfi.badw.de.

The code can be kept rather simple and is illustrated first for the *normalized* Legendre functions. Let PNM be a vector array of sufficient length that contains on input the values of normalized Legendre functions, complete up to maximum degree and order NMAX, with following sequence $P_{00}, P_{10}, P_{11}, P_{20}, P_{21}, P_{22}, P_{30}, P_{31}$... Then derivatives for all degrees and orders with respect to colatitude θ are computed and stored in a second vector array, DPNM, by the following FORTRAN statements.

```
ia = 1
dpnm2= PNM(2)
do n = 1,NMAX
   ia = ia + n
   temp = PNM(ia)
   DPNM(ia) = - sqrt(dble( ia-1 ))*PNM(ia+1)
   fac1 = sqrt(dble( 2*(n+1)*n ))
   do m = 1,n-1
      i = ia + m
      fac2 = sqrt(dble( (n-m)*(n+m+1) ))
      deriv = fac1*temp - fac2*PNM(i+1)
      temp = PNM(i)
      DPNM(i) = 0.5d0*deriv
      fac1 = fac2
   end do
   DPNM(ia+n) = sqrt(dble(n)/2.d0)*temp
end do
DPNM(3) = dpnm2
```

The sequence of computations has been arranged such that the arrays PNM and DPNM may share the same memory. Thus, the two vector arrays could be given an identical name. However, it is more general, to keep the different names in the code and let the two array names appear as formal arguments of the subroutine. The memory for the two arrays can then be shared by simply using the same actual parameter.

Here is the code for the *unnormalized* Legendre functions

```
ia = 1
do n = 1,NMAX
   ia = ia + n
   temp = PNM(ia)
   DPNM(ia) = - PNM(ia+1)
   do m = 1,n-1
      i = ia + m
      fac = dble( (n+m)*(n-m+1) )
      deriv = fac*temp - PNM(i+1)
      temp = PNM(i)
      DPNM(i) = 0.5d0*deriv
   end do
   DPNM(ia+n) = dble(n)*temp
end do
```