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Zeros of Legendre polynomial for high order Gauss-Legendre quadrature*

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सार — इस लेख में कोज्या θ तथा θ को आधारभूत चरांक मानकर लेजान्ड्रे बहुपद के अभिकलन के लिये निकटवर्ती त्रुटि संचरण पर विचार-विमर्श किया गया है। द्विघाती अभिसारी न्यूटन-राफ्सन विधि पर आधारित लेजान्ड्रे बहुपद के सभी शून्यों के अभिकलन के लिये θ को आधारभूत चरांक मान कर एक पुनरावृति योजना प्रस्तुत की गई है तथा विभिन्न उपयुक्त स्थिर सम्बन्धों का उपयोग कर उनकी परिशुद्धता सुनिश्चित की गई है।

ABSTRACT. Roundoff error propagations in the computation of Legendre polynomial with cos θ and θ as the basic variables are discussed. An iterative scheme with θ as the basic variable, for computing all the zeros of Legendre polynomial based on the quadratic convergent Newton-Raphson method is presented and their accuracy is determined by using different appropriate invariant relations.

1. Introduction

In majority of the present spectral models of the atmosphere (Bourke 1972, 741 ; Machenhauer *et al.* 1972 and others), the transform method as developed independently by Orszag (1970) and Eliassen *et al.* (1970) is used for obtaining the spectral representation of non-linear terms. In the models where spherical harmonics are chosen for spectral representations of the variables, the transform method involves the Legendre transforms of non-linear terms along the meridional direction. The meridional integration can be numerically performed exactly by using a Gauss-Legendre quadrature formula of appropriate order. An idea of the high order of Gauss-Legendre quadrature formula required in the models may be easily understood from the following example. A high resolution spectral model with the rhomboidal truncation at wave number 30, generally preferred for extended range prediction and other experiments, uses the Gauss-Legendre quadrature formula of order 76, which is quite high.

The abscissas of Gauss-Legendre quadrature formulae are the zeros of Legendre polynomial. Among the few problems that arise in the numerical computations, the most serious one is the presence of large errors in the computed values of the polynomial and its derivatives. This is due to the utilisation of polynomial expansions, which limits strongly the accuracy of the zeros.

One of the main purposes of this study is to identify a suitable procedure for minimising the errors. Another important problem associated with the use of Newton-Raphson iterative method for finding the zeros is the converging of many initial approximations of the zeros to a single value in the course of iteration. One way to avoid this problem is to choose the initial approximations quite close to the exact values. Other possible solution of this problem is to use the alternative method (Aberth 1973) specially developed for this purpose. In this paper we have chosen first alternative and same is discussed.

2. Choosing the basic variable

The normalised Legendre polynomial of degree n, *i.e.*, $P_n(\cos\theta)$, can be expressed in the form :

$$P_n(\cos\theta) = C_n \sum_{j=0}^{J} a_{n-2j} (\cos\theta)^{n-2j} \tag{1}$$

where,

$$C_n = \frac{1.3.5\ldots(2n-1)}{n!} \sqrt{\frac{2n+1}{2}} \tag{1a}$$

$a_n = 1,$

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TABLE 1

Values of C_n and $\sum_{j=1}^{J} |a_{n-2j}|$ for Legendre polynomials of various degrees n

Degree of the polynomial n	C_n	$\sum_{j=1}^{J} \| a_{n-2j} \|$
30	8.60×10^{8}	2.61×10^{2}
35	2.75×10^{10}	6.70×10^{2}
40	8.80×10^{11}	1.72×10^{3}
45	2.82×10^{13}	4.40×10^{3}
50	9.01×10^{14}	1.13×10^{4}
55	2.88×10^{16}	2.89×10^{4}
60	9.22×10^{17}	7.41×10^{4}
65	2.95×10^{19}	1.90×10^{5}
70	9.44×10^{20}	4.87×10^{5}
75	3.02×10^{22}	1.25×10^{6}
80	9.66×10^{23}	3.20×10^{6}
85	3.09×10^{25}	8.20×10^{6}
90	9.89×10^{26}	2.10×10^{7}
95	3.16×10^{28}	5.39×10^{7}
100	1.01×10^{30}	1.38×10^{8}

$$a_{n-2j} = (-1)^j \frac{n(n-1)\ldots(n-2j+1)}{2^j j!\,(2n-1)(2n-3)\ldots(2n-2j+1)} \quad \text{for } j=1,2,\ldots\ldots J \qquad (1b)$$

and θ is the co-latitude, $J = \frac{n}{2}$ for even n and

$$J = \frac{n-1}{2}$$

for odd n. In order to save computation time the normalisation constant C_n and the expansion coefficients $a_n, a_{n-2}, \ldots\ldots, a_{n-2j}$ are computed from the following recursion relations, which can be easily derived from Eqns. (1a) and (1b) respectively as

$$C_k = 2\sqrt{1-\left(\frac{1}{2k}\right)^2}\; C_{k-1} \quad \text{for } k=1,2,\ldots\ldots,n \qquad (2a)$$

and

$$a_{n-2j} = -\frac{(n-2j+2)\,(n-2j+1)}{2j(2n-2j+1)}\, a_{n-2j+2}$$

$$\text{for } j=1,2,\ldots\ldots,J \qquad (2b)$$

It follows from Eqn. 2(a) that $C_k/C_{k-1} = 2 \geqslant 1$ for $k=1,\ldots\ldots,n$; this condition leads to the amplification of roundoff error in course of its propagation during the computation of C_n. Further more, $C_n \approx 2^{n-1}$ which is quite large for a sufficiently large value of n. This situation is also favourable for subsequent large amplification of the errors of the expansion coefficients, thus contributing to the gross error in the computaion of $P_n(\cos\theta)$.

It can be seen from the recursion relation (2b) that the ratio

$$\left| \frac{a_{n-2j}}{a_{n-2j+2}} \right|$$

is a monotonic decreasing function of j for fixed n and having values greater than unity for the first few values of j. Furthermore, majortity among the expansion coefficients are having magnitude far greater than unity. This situation is also favourable for the amplification of the roundoff errors in course of their propagation, thus, contributing to the net computation error of Legendre polynomials. It is expected that the maximum upper limit to the net computation error of P_n due to the presence of inherent roundoff error ϵ is proportional to :

$$C_n\epsilon \sum_{j=0}^{J} \left| a_{n-2j} \right|. \text{ The values of } C_n \text{ and } \sum_{j=0}^{J} \left| a_{n-2j} \right|$$

for $n=30, 35, \ldots\ldots 100$ are given in Table 1. In the actual computation the error is noticed to be near to the factor $C_n\epsilon$ than the product

$$\epsilon\, C_n \sum_{j=0}^{J} \left| a_{n-2j} \right|. \text{ This behaviour of the error}$$

is due to the following reasons. C_n is dominating factor compared to the second factor as seen from the table. The contribution from the second factor appeared as the weighted sum of roundoff errors, which is most likely to be much less than its maximum upper limit

$$\epsilon \sum_{j=0}^{J} \left| a_{n-2j} \right|$$

In brief, we can say that the polynomial expansion of $P_n(\cos\theta)$ is not suitable for the computations because of poor roundoff error characteristic for higher n. The number of significant digits in the computed value decreases rather fast with the increase of n. For this reason we preferred to use the expression for Legendre polynomial and its first derivative, which involves multiples of θ, instead of the powers of $\cos\theta$. They are :

$$P_n(\cos\theta) = D_n \sum_{j=0}^{J} b_{n-2j} \cos(n-2j)\theta \qquad (3)$$

$$\text{and } \frac{dP_n}{d\theta} = -D_n' \sum_{j=0}^{J'} b'_{n-2j} \sin(n-2j)\theta \qquad (4)$$

where the normalisation constant D_n is given by

$$D_n = \frac{1.3\ldots(2n-1)}{n!\,2^{n-1}} \sqrt{\frac{2n+1}{2}} \qquad (5a)$$

the coefficients $b_n, b_{n-2}, \ldots\ldots b_{n-2j}$ are given as

$$b_{n-2j} = \frac{1.3\ldots(2j-1)\,n(n-1)\ldots(n-j+1)}{j!\,(2n-1)(2n-3)\ldots(2n-2j+1)}$$

$$\text{for } j=0,1,\ldots\ldots J \qquad (5b)$$

b'_{n-2j} and D_n' can be expressed in terms of b_{n-2j} and D_n respectively as

$$b'_{n-2j} = \frac{(n-2j)}{n} b_{n-2j} \qquad (5c)$$

$$D'_n = n\, D_n$$

where $J' = J-1$ for even n and $J' = J$ for odd n.

In cases when n is even, the last term of Eqn. (4) is to be multiplied by a factor $\frac{1}{2}$. Belousov (1962) has studied the roundoff error characteristics of Eqns. (3) and (4) and has proposed algorithms for calculating the normalisation constant D_n and the expansion coefficients $b_n, b_{n-2} \ldots, b_{n-2j}$ based on the recursion relations. His algorithms have the property of damping the propagation of roundoff error and they are briefly discussed below for an easy comparison with the algorithms based on Eqn. (1).

The recursion relations for computing D_n and the coefficients can be easily obtained from Eqns. (5a) and (5b) respectively as follows :

$$D_k = \sqrt{1 - \left(\frac{1}{2k}\right)^2}\, D_{k-1} \text{ for } k=1,\ 2, \ldots, n \qquad (6a)$$

and

$$b_{n-2j} = \left[1 - \frac{n-2j+1}{j(2n-2j+1)}\right] b_{n-2j+2} \text{ for } j=1, 2, \ldots, J \qquad (6b)$$

The following inequalities are easily followed from Eqns. (6a) and (6b).

$$\frac{D_k}{D_{k-1}} < 1 \quad \text{for } k=1, 2, \ldots, n,$$

and

$$\frac{b_{n-2j}}{b_{n-2j+2}} < 1 \quad \text{for } j=1, 2, \ldots, J.$$

It is implied by these inequalities that the roundoff errors in the computation of D_n and the coefficients b_n, b_{n-2}, $\ldots$, b_{n-2j} are damped in course of their propagations. More or less the same error characteristics are observed for D'_n and the coefficients $b'_{n-2}, \ldots, b'_{n-2j}$, involved in computation of $dP_n/d\theta$ from Eqn. (4).

A comparison in respect of the computational error characteristics between the two representations of Legendre polynomial immediately lead to the conclusions that the second is far superior to the first. It seems natural to work with the θ as the basic variable for computations of P_n and $dP_n/d\theta$ by using Eqns. (3) and (4) respectively.

3. Newton-Raphson's method and the initial approximations

We have chosen in this study the Newton-Raphson iterative method for finding simultaneously all the zeros of Legendre polynomial of high degree. This method is quadratic in convergence and is easily adoptable to the computers. In some cases many different initial approximations of the zeros converge to a single value, when the initial approximations are not close enough. In general, convergence to a multiple zero is slower compared to a simple zero. It may be mentioned here that all zeros of P_n are simple and real and their close initial approximations to the exact values can be easily obtained.

Let θ_1, θ_2, $\ldots$, θ_n be the initial approximations to the zeros of P_n and $\theta_1+\triangle\theta_1, \ldots, \theta_n+\triangle\theta_n$ are the modified approximations after the end of first iteration. In the Newton-Raphson method $\triangle\theta_l$ is given by :

$$\triangle\theta_l = -P_n(\cos\theta_l)/\frac{dP_n}{d\theta}(\cos\theta_l)$$

where $l=1, 2, \ldots n$.

The zeros lie in the interval $0 < \theta < \pi$ and are symmetric around the line $\theta=\pi/2$; further, for odd n one of the zeros lies on this line. Only the zeros, J in number, that lie in the half interval $0 < \theta < \pi/2$, need to be computed explicitly the remaining zeros are obtained on symmetric consideration.

To start Newton-Raphson iteration process for computing simultaneously all the zeros of Legendre polynomial, good initial approximations to their exact values are required. For this purpose many formulae are available in the literature but we preferred the following formula due to Szego (1936):

$$\theta_l = \frac{\pi}{2}\left[\frac{l-\frac{1}{2}}{n} + \frac{l}{n+1}\right] \qquad (8)$$

where, $l=1, 2, \ldots, J$

This approximation provides the zeros accurate up to three decimal places. The more accurate approximations than (8) are available but they require more computation time. In actual computation, no problem was encountered in using Eqn. (8) as the initial approximations.

For terminating the iteration process, an upper limit to the convergence error is prescribed. This value depends upon the computer accuracy, for computer with 48 bits word representation we selected the value 10^{-10}. It is noticed that not more than 4 iterations are required for the convergence of the iterative procedure.

4. Accuracy of computation

In this section we will discuss a procedure for determining the accuracy of the computed zeros of P_n, *i.e.*, the minimum number of decimal places upto which each of the computed values is correct. The procedure consists of using different suitable invariant relations, such that, their numerical evaluation involves the zeros, then determining upto what accuracy these invariant relations are satisfied. This procedure is expected to provide an upper bound of possible error in the computed zeros. The computation error of zero is composed of two components — one is due to the machine inherent roundoff error and the other is due to the truncation error of the iterative method. It is easily followed from the previous discussion on the propagation characteristic of roundoff error of the numerical algorithms based on Eqn. (3) that the truncation error component is much larger than the roundoff error component.

One of the invariant relations considered here involves the Gaussian weight given by

$$G_l = \frac{(2n-1)\sin^2\theta_l}{[nP_{n-1}(\cos\theta_l)]^2} \tag{9}$$

where $l=1, 2, \ldots. J$ and G_l is the Gausian weight. It is obvious from Eqn. (9) that the Gaussian weights are positive and symmetric around $\theta=\pi/2$. Further, they satisfy the following invariant condition :

$$\sum_{l=1}^{n} G_l = 2 \tag{10}$$

The other invariant relations are provided by the following orthonormal properties of Legendre polynomial.

$$\int_{-1}^{1} P_m P_m \, dx = 1 \tag{11}$$

and

$$\int_{-1}^{1} P_{m1} P_{m2} \, dx = 0, \quad \text{for } m_1 \neq m_2 \tag{12}$$

where $x = \cos\theta$.

Integrals (11) and (12) can be evaluated exactly by using a Gauss-Legendre quadrature formula of sufficient order; the n-points formula is exact for the polynomial of degree $2n-1$ and less (Kopal 1955, Krylove 1962). Integrand in Eqn. (11) is a polynomial of degree $2m$, while that in Eqn. (12) it is of degree (m_1+m_2).

For determing the lower limit of accuracy of the n computed zeros, the Gauss-Legendre quadrature formula of order n, whose abscissas are these zeros, is used for evaluating integrals (11) and (12). In integral (11), m is assigned a single value, whereas in integral (12) three different combinations of m_1 and m_2 are chosen. Values of m, m_1 and m_2 are so chosen as to satisfy the conditions $2m \leqslant (2n-1)$ and $(m_1+m_2) \leqslant (2n-1)$. Thus, for each n, the five invariant relations are used for the purpose mentioned above and this number is considered to be sufficient.

Computation error in each numerical evaluation of the invariant relation is the weighted sum of the errors in zeros as can be easily concluded from Eqns. (10)-(12). We have calculated all the zeros of Legendre polynomial of degree varying from 1 to 100. In all, nearly 500 invariant relations are checked for finding the minimum degree of accuracy of the computed zeros. A sample of 500 errors is large enough to provide an upper bound of the error in zeros which is equal to the maximum absolute error of the sample. It is concluded from the result so obtained that the computed zeros are atleast correct to first 8 decimal places or in other words almost only two decimal places are lost in the process of computation.

Finally, we determined the exact number of decimal places to which the zeros are correct by repeating the complete calculations in double-precision arithmetic. The zeros obtained by using double-precision computation are truncated to get the correct zeros to the decimal places involved in single-precision arithmetic. These values are compared against the values obtained from single-precision computation. It is found that the values are having 9 decimal place accuracy.

5. Conclusion

The numerical algorithms based on the representation of Legendre polynomial and its derivative in terms of cos θ, have been analysed for the roundoff error propagation in course of their computations. Results of this analysis have been compared with those obtained with the representation based on θ as the basic variable. It has been concluded, on the basis of the comparison, that only with the use of numerical algorithms based on θ as the basic variable, it is possible to compute the zeros sufficiently accurate, particularly in the cases of high degree polynomials.

It has been shown that the Newton-Raphson iterative method can be easily adopted for the representation in terms of θ. It has been found that only one decimal place was lost in the computation of the zeros of P_n for $n \leqslant 100$.

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