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NUMERICAL INTEGRATION WITH LINEAR COMBINATION OF CHEBYSHEV–GAUSS QUADRATURES

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Summary

A numerical integration method based on a special combination of the two Chebysev-Gauss quadratures is presented. This procedure enables us to determine the bound for error of the calculated value starting from the quadratures series themselves.

1. Introduction

The most problematical part of numerical integration is the determination of bound for error. Using any quadrature formula,the calculation of bound for error demands the knowledge of some higher order derivate of the function to be integrated. The error can be estimated only if this derivative is bounded in the domain of integration, and if this bound can be calculated. Owing to this circumstance the error estimation of the quadrature formulae, especially that of the higher order ones (e.g. Gaussian type quadratures) is rather cumbersone.

The error can be reduced by dividing the integration domain into sections and using some lower precision formula for the sections separately. Thus it is possible to reduce the bound for error without the necessity of estimating higher derivates of the function. Among these methods the simplest one is the trapezoidal rule, but even then a bound is a needed for the second derivative, and it is still to be feared that the calculated bound for error will be too high. In case of integrations requiring high precision another problem arises from the computations: summing up numerous terms the rounding errors may reach a significant amount.

But the main difficulty of the task of numerical integration is that we have to know too much information concerning the function to be integrated, e.g. we have to know the bounds of its higher order derivatives. In case of practical problems serious difficulties arise in the calculation of these quantities or it is even impossible to obtain them.

Now we will present a method where no derivatives have to be known for the estimation of errors, yet it is applicable to a relatively large class of functions. The essence of the method can be reviewed briefly as follows. Let the function be differentiable continuously five times in a finite interval. We approximate the integral I of function f for this interval by two Gaussian type quadrature series, using an increasing number of points. Let these be denoted by $\{C_n\}$ and $\{S_n\}$, respectively. For the elements of the chosen class of functions and for the chosen quadrature series we have

$$S_n < I < C_n \quad \text{or} \quad C_n < I < S_n$$

when n exceeds some threshold index N. The convex combination of the two series forms a new series converging to I:

$$I_n = \alpha C_n + (1-\alpha) S_n, \qquad 0 \le \alpha \le 1.$$

Owing to some order of magnitude relations concerning C_n and S_n, the error can be estimated as follows:

$$|I - I_n| < |C_n - S_n|.$$

We will also determine the number α for which the order of convergence of the linear combination is maximum.

2. Notations

Let T_n denote the Chebyshev polynomal of first kind:

$$T_n(x) = \cos(n \arccos x), \quad n = 0, 1, \ldots, \quad x \in [-1, 1],$$

t_{nk} the zeros of the polynomial:

$$t_{nk} = \cos \frac{2k-1}{2n}\pi, \quad k = 1, 2, \ldots, n$$

We denote the Chebyshev polynomal of second kind by U_n:

$$U_n(x) = \frac{\sin(n \arccos x)}{\sin(\arccos x)}, \; n = 1, \ldots, \; x \in (-1, 1),$$

and its zeros by u_{nk}:

$$u_{nk} = \cos \frac{k}{n}\pi, \quad k = 1, 2, \ldots, n-1.$$

The integral of the function f, its Chebyshev-Gauss quadratures calculated with the Chebyshev polynomals of first and second kind are the following:

$$I = \int_{-1}^{1} f(x)dx,$$

$$C_n = \frac{\pi}{n} \sum_{k=1}^{n} f(t_{nk}) \cdot \sqrt{1 - t_{nk}^2},$$

$$S_n = \frac{\pi}{n} \sum_{k=1}^{n-1} f(u_{nk}) \cdot \sqrt{1 - u_{nk}^2}, \; n = 2, 3, \ldots$$

Theorem. *In case the function f is five times continously differentiable within the interval* $[-1, 1]$, *1) there exist such a threshold N that*

$$|I - \frac{2}{3}C_n - \frac{1}{3}S_n| < |C_n - S_n|, \quad \text{if } n > N,$$

2) among the convex combinations

$$\{\alpha C_n + (1-\alpha)S_n\}, \qquad 0 \le \alpha \le 1$$

the order of convergence for $\alpha = 2/3$ *is* $O(1/n^4)$*, while that in the other case is* $O(1/n^2)$.

Proof. The theorem will be proved first for the Chebyshev polynomials of second kind, then for the series of the function f expanded in terms of Chebysev polymials of second kind.

a) Let us take $f = U_{2m-1}$, $m = 1, 2, \ldots$ the Chebyshev polynomial of even index is an odd function, therefore its integral and its approximative values vanish. Let us denoted by the index m the integral of U_{2m-1} as well as its approximative values. Then we have :

$$I_m = \int_{-1}^{1} U_{2m-1}(x)dx = \int_{0}^{\pi} \sin(2m-1)x dx = \frac{2}{2m-1},$$

$$C_{nm} = \frac{\pi}{n} \cdot \sum_{k=1}^{n} \sin(2m-1)\frac{2k-1}{2n}\pi = \frac{\pi}{n} \cdot \frac{1}{\sin\frac{\pi}{2n}(2m-1)},$$

$$S_{nm} = \frac{\pi}{n} \cdot \sum_{k=1}^{n-1} \sin(2m-1)\frac{k}{n}\pi = \frac{\pi}{n} \cdot \text{ctg}\frac{\pi}{2n}(2m-1).$$

If we have $n \ge m$, then

$$S_{nm} < I_m < C_{nm},$$

because

$$C_{nm} - I_m = \frac{2}{2m-1} \cdot \frac{\frac{\pi}{2n}(2m-1) - \sin\frac{\pi}{2n}(2m-1)}{\sin\frac{\pi}{2n}(2m-1)} > 0,$$

and

$$S_{nm} - I_m =$$
$$= \frac{2}{2m-1} \frac{\frac{\pi}{2n}(2m-1)\cos\frac{\pi}{2n}(2m-1) - \sin\frac{\pi}{2n}(2m-1)}{\sin\frac{\pi}{2n}(2m-1)} < 0$$

if

$$0 < \frac{\pi}{2n}(2m-1) < \pi.$$

Thus, for any convex combination of the approximative sums C_{nm} and S_{nm} the estimation

$$|I_m - \alpha C_{nm} - (1-\alpha)S_{nm}| < |C_{nm} - S_{nm}|$$

is valid for $n \geq m$. The order of convergence of the series $\{C_{nm}\}$ and $\{S_{nm}\}$ is $O(1/n^2)$, while the same for the series $\{\frac{2}{3}C_{nm} + \frac{1}{3}S_{nm}\}$ is $O(1/n^4)$. These orders of magnitude are shown by the following limits :

$$\lim_{n\to\infty} n^2(C_{nm} - I_m) = \frac{\pi^2}{12}(2m-1),$$
$$\lim_{n\to\infty} n^2(S_{nm} - I_m) = -\frac{\pi^2}{6}(2m-1), \qquad (*)$$
$$\lim_{n\to\infty} n^4(\frac{2}{3}C_{nm} + \frac{1}{3}S_{nm} - Im) = \frac{\pi^4}{1440}(2m-1)^3.$$

b) Now let us take

$$f(x) = \sum_{m=1}^{\infty} a_m U_{2m-1}(x), \qquad \text{where}$$

$$a_m = \frac{2}{\pi}\int_{-1}^{1} \sqrt{1-x^2}\, f(x) U_{2m-1}(x)dx$$

Since f is five times continously differentiable on the interval $[-1,1]$, we have $a_m = O(1/m^5)$.

Thus, the integral and the approximative sums are:

$$I = \int_{-1}^{1} f(x)dx = \sum_{m=1}^{\infty} a_m I_m ,$$

$$C_n = \sum_{m=1}^{\infty} a_m C_{nm} , \quad S_n = \sum_{m=1}^{\infty} a_m S_{nm} .$$

Since $a_m = O(1/m^5)$, the three series are absolutely convergent.

To prove the theorem we have see only that there exist a number N such that the quantity I is between the series C_n and S_n, i.e. we have

$$(C_n - I)(S_n - I) < 0, \quad \text{if } n > N.$$

For this it is sufficient to show that the second term of the right side of the equality

$$S_n - I = -2(C_n - I) + 3(\frac{2}{3}C_n + \frac{1}{3}S_n - I)$$

converges towards zero in higher order of magnitude than the expression on the left side.

The limits showing the order of magnitude can be calculated like those under (*), since the limit sign and the summations are interchangeable owing to the absolute convergence.

$$\lim_{n\to\infty} n^2(C_n - I) = \lim_{n\to\infty} n^2 \left[\sum_{m=1}^{\infty} a_m C_{nm} - \sum_{m=1}^{\infty} a_m I_m\right] =$$

$$= \sum_{m=1}^{\infty} a_m \lim_{n\to\infty} n^2(C_{nm} - I_m) = \frac{\pi^2}{12} \sum_{m=1}^{\infty} a_m (2m-1).$$

Likewise we have:

$$\lim_{n\to\infty} n^2(S_n - I) = -\frac{\pi^2}{6}\sum_{m=1}^{\infty} a_m(2m-1),$$

$$\lim_{n\to\infty} n^4\left(\frac{2}{3}C_n + \frac{1}{3}S_n - I\right) = \frac{\pi^4}{1440}\sum_{m=1}^{\infty} a_m(2m-1)^3.$$

3. Conclusion

A similar theorem can be started for the same 2/3 to 1/3 linear combination of quadrature of series of Gauss type defined with the so called "shifted" Chebyshev polynomials. The definition of these polynomals is :

$$T_n^*(x) = T_n(2x-1), \qquad U_n^*(x) = U_n(2x-1).$$

The zeros of T_n^* are :

$$t_{nk}^* = \cos^2\frac{2k-1}{2n}\pi, \qquad k = 1,\ldots,n$$

and the same for U_n^* are:

$$u_{nk}^* = \cos^2\frac{k}{2n}\pi, \qquad k = 1,\ldots,n-1$$

The integral of the function f and the quadratures according to T_n^* and U_n^* are respectively:

$$I = \int_0^1 f(x)dx,$$

$$C_n^* = \frac{\pi}{n}\sum_{k=1}^{n} f(t_{nk}^*)\cdot\sqrt{t_{nk}^*(1-t_{nk}^*)},$$

$$S_n^* = \frac{\pi}{n}\sum_{k=1}^{n-1} f(u_{nk}^*)\cdot\sqrt{u_{nk}^*(1-u_{nk}^*)}.$$

When the function f is five times continuously differentiable on the interval $[0,1]$, then the same holds for the quadrature series $\{C_n^*\}$ and $\{S_n^*\}$ as we have proved for the Chebyshev-Gauss polynomials. Among their linear combinations the one defined as

$$\{\frac{2}{3}C_n^* + \frac{1}{3}S_n^*\}$$

approximates the true value of integral in a higher order of magnitude than the other ones, and the error can be estimated in a similar manner:

$$|I - \frac{2}{3}C_n^* - \frac{1}{3}S_n^*| < |C_n^* - S_n^*|, \quad \text{if } n > N.$$

For a proof let us write down the integral of U_{2m-1}^* and the C_{nm}^* and S_{nm}^* approximative sums as well. Using the definition of U_{2m-1}^*, the following equalities can be verified:

$$2 \cdot \int_0^1 U_{2m-1}^*(x)dx = \int_{-1}^1 U_{2m-1}(x)dx,$$

$$2C_{nm}^* = C_{nm}, \qquad 2S_{nm}^* = S_{nm},$$

$$m = 1,2,\ldots, \qquad n = 2,3,\ldots.$$

4. Example

The surprisingly fast convergence of the $\frac{2}{3}$ to $\frac{1}{3}$ combination of the Chebyshev-Gauss quadratures has been observed in solving lots of problems. Now we will show the advantages of the method in an example.

The problem con be found in the book af Anthony Ralston : Introduction to the numerical analysis, in the chapter discussing the choice of quadrature methods. The integral in question to ten significant digits, is:

$$\int_{-4}^{4} \frac{1}{1+x^2} dx = 2\text{arctg}4 = 2{,}651635327.$$

The problem shows that the accuracy cannot be improved arbitrarily with the help of higher order Newton-Cotes formulae (owing to the rapid increase of derivatives). For the solution of the above problem the book suggests the use of methods which divide the interval in parts, e.g. the trapezium and Simpson formulas.

The table shows that linear combination of Chebyshev-Gauss quadratures assures a much faster convergence than those mentioned above. (For the sake of clarity we have underlined the correct decimal.) E.g. In case of the Simpson formula, assuming 35 points of division, the error is $2{,}8 \cdot 10^{-6}$, while the error of I_n is $1{,}3 \cdot 10^{-8}$ at the same time.

The table shows also that the series C_n approximates the true value from above, while S_n does it from below. (The series C_n^* and S_n^* not contained in the table for the sake of space saving show a similar behaviour.) The bound for error calculated from their difference is $7{,}9 \cdot 10^{-5}$ for 35 points. With the Simpson formula the same number amounts to $3{,}3 \cdot 10^{-3}$, but for the determination of this we had to compute the bound $\max |f^{IV}| = 24$.

It is worth mentioning the high relative accuracy of I_n^* despite the low number of points the difference between I_n^* and I_n diminishes. Bot phenomena can be observed in case of a lot of problems. But it is perhaps more important to note what the example shows concerning the relation between the Romberg method and I_n. (The library programs of numerical integration generally apply Romberg-Type methods.) In high precision computations, up to some 20 significant digits, the accuracy of the Chebyshev-Gauss series is generally higher than that of the Romberg method if we use the same number of points.

Number of base points n	Newton-Cotes formula of n^{th} order	Trapezium formula	Romberg method	Simpson formula	C_n	S_n	$I_n = \frac{2}{3}C_n + \frac{1}{3}S_n$	I_n^*
3	5,490	4,2353	5,4902	5,4902	4,5110	1,4510	3,4910	2,6803
5	2,278	2,9176	2,2776	2,4784	3,2366	2,1487	2,8740	2,6491
7	3,329	2,7005		2,9084	2,8584	2,4532	2,7234	2,65179
9	1,941	2,6588	2,5836	2,5725	2,7279	2,5747	2,6768	2,651638
11	3,596	2,6511		2,6953	2,6805	2,6214	2,6608	2,651641
:								
17		2,65051	2,65420	2,64773	2,65370	2,64891	2,65210	2,651637
:								
29		2,65125903		2,65159874	2,65186874	2,65117186	2,65163645	2,65163549
31		2,65130749		2,65165039	2,65183779	2,65123153	2,65163570	2,65163545
33		2,65134717	2,65186284	2,65162726	2,65181332	2,65127966	2,65163543	2,65163542
35		2,65138005		2,65163808	2,65179332	2,65131936	2,65163534	2,65163540
:								
61		2,65155332		2,651635265	2,651687314	2,651531330	2,651635319	2,651635337
63		2,65155853		2,651635275	2,651684066	2,651537833	2,651635322	2,651635334
65		2,65156325	2,65163060	2,651635281	2,651681117	2,651543734	2,651635323	2,651635333

Summing up, we can form the following statements concerning the approximative series calculated as linear combinations of Chebyshev-Gauss quadratures. For their application it is sufficient to know that the integrand is differentiable five times on the interval of integration. The computation of the approximative value and of the bound for error is very simple. Finally it is to be mentioned that these integral-approximating series show generally a very quick convergence,as we have shown in the example above.

References

[1] STOER, J. BURLISCH, R. Introduction to Numerical analysis, Spinger Verlag, New York Inc. 1980

[2] RALSTON, A. A First Course in Numerical Analysis , McGraw-Hill 1965

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