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Gaussian Quadrature of Integrands Involving an Imaginary Error Function

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Abstract

Analytical polynomials corresponding to the weight function erfi (z) and defined on the complex plane are obtained. Abscissas and weight factors for the associated Gaussian Quadrature are then deduced (up to 12 – points formulas). In previous recent research papers already discussed the computation of Accuracy of Asymptotic Error. To test the efficiency of the new gaussian rule from the example.

Keywords: Imaginary Error function, Analytical polynomial, Gaussian Quadrature.

Introduction

In previous research papers so much work done on the field of quadrature and discovered the new different source of fields. To obtain an approximation to a definite integral for tabulated functions with arbitrary grid spacing, cubic spline integrators supply and closed curve intervals an efficient way [2]. It extremely interesting to needed for evaluation of few integrands by Gaussian Quadrature formula [4]. Somewhere little known about the integrand such as adaptive quadrature method can be used for high probability of success [3]. The most useful advantage seen to be there in time consuming condition for computation of integrand. Considered the integrations on some weight function and intervals have been so far [4] – [6]. Nowadays the paper represents that the Gaussian Quadrature formula constructed for calculating the expression of the type

$$I = \int_0^\infty erfi(z) f(z) dz \qquad (1)$$

where, $erfi(z) = -i\ erf(iz)$ and i is the imaginary unit.

Therefore, $$erf(iz) = \frac{2}{\sqrt{\pi}} \int_0^{iz} e^{-t^2}\ dt \qquad (2)$$

Hence $$erfi(z) = -\frac{2i}{\sqrt{\pi}} \int_0^{iz} e^{-t^2}\ dt \qquad (3)$$

is the imaginary error function and f(z) being the analytic function.

To construct the abscissas z_i and weight factors w_i appearing in the Gaussian expression [1]

$$I \approx \sum_{i=1}^{n} w_i f(z_i) \qquad (4)$$

It is necessary to find the set of orthogonal polynomials $\emptyset_k$, k = 0, 1, 2…, n, and

$< \emptyset_i, \emptyset_j > = 0\ \ if\ i \neq j$, corresponding to the following inner product

$$< f,g > = \int_{-\infty}^{\infty} erfi(z)f(z)g(z)\,dz \qquad (5)$$

Analytical Polynomial and Gaussian Formula: The Gramm Schimdt orthogonalization can be used to generates these polynomials from the set of non-orthogonal functions

$$1, z, z^2, z^3, \ldots.., z^n. \qquad (6)$$

This procedure is describing in [7] and the amount to determining recursively the polynomials $\emptyset_k(z)$ through the following relation

$$\emptyset_k(z) = 1 \qquad (7)$$

$$\emptyset_k(z) = z^k - \sum_{n=0}^{k-1} \frac{\int_0^{\infty} erfi(t)t^k\, \emptyset_n(t)dt}{\int_0^{\infty} erfi(t)\,(\emptyset_n(t))^2 dt}\, \emptyset_n(z), \qquad (8)$$

where k = 1, 2, 3, ……, n.

If the explicit expression for these polynomials

$$\emptyset_k(z) = \sum_{j=0}^{k} \emptyset_j^k\, z^j \qquad (9)$$

is above shown in (6) and (7), the following expression is obtained

$$\sum_{n=0}^{k} \emptyset_n^k\, z^k = z^k - \sum_{n=0}^{k-1} \frac{\sum_{i=0}^{n} \emptyset_i^n \mu_{i+k}}{\sum_{l=0}^{n}\sum_{i=0}^{n} \emptyset_i^n \emptyset_l^n \mu_{i+1}} \sum_{j=0}^{n} \emptyset_j^n\, z^j \qquad (10)$$

Where μ_p are the moments of the weight function

$$\mu_p = \int_{-\infty}^{\infty} erfi(z)z^p\, dz = \frac{\tau(\frac{p}{2}+1)}{\sqrt{\pi}(p+1)} \qquad (11)$$

In Eq. (10), the right-hand side can be put under an explicit polynomial form, by re-ordering the summation on n and j. This leads to the following recursion relations for computing the coefficients $\emptyset_j^k$ of the orthogonal polynomials.

$$\emptyset_k^k = 1 \qquad (12)$$

And, for n ≠ k

$$\emptyset_n^k = -\sum_{j=n}^{k-1} \frac{\sum_{i=0}^{j} \emptyset_i^j \mu_{i+k}}{\sum_{i=0}^{j}\sum_{l=0}^{j} \emptyset_i^j \emptyset_l^j \mu_{i+l}}\, \emptyset_n^j. \qquad (13)$$

The ill-conditioned character is seen in the past literature for the Gaussian Rule [8]-[11] to the problems of finding the zeros and weights. Equation (13) is not possible in general case about to forecast the stability and which has two different facts of aspects. If μ_k is the moment which has exactly known quantities, the recursion scheme can propagate the truncation error that affects the coefficients $\emptyset_j^k$ at each stage of the recursive process while the polynomial coefficients may be sensitive to errors introduced in computing the moments μ_p. It reduces the accuracy of the computed coefficients in the progressive form of effective act on both. Furthermore, it gives error when the time of construction of zeros of polynomial and the weight function which given. For this reason, an arithmetic of about 35 figures has been used in performing the computation realized here and a check on the μ-wise sensitivity of the polynomial coefficients, as well as the abscissas and weight factors, has been completed.

Table 1

Sensitivity of 12th -degree analytic polynomial to a slight variation of a moments μ_p. A relative increase of 3.10^{-33} of all moments has been performed. $\frac{\nabla\emptyset_{12}^i}{\emptyset_{12}^i}$ is the relative change of the polynomial coefficients, $\frac{\nabla z_i}{z_i}$ is the relative change of its zeros, and $\frac{\nabla w_i}{w_i}$ is the corresponding relative change in the weight factor. [1]

i	$\left\|\frac{\nabla\emptyset_{12}^i}{\emptyset_{12}^i}\right\|$	$\left\|\frac{\nabla z_i}{z_i}\right\|$	$\left\|\frac{\nabla w_i}{w_i}\right\|$
1	(-16) 3.4	(-17) 3.7	(-17) 3.6
2	(-16) 3.0	(-17) 3.7	(-17) 2.9
3	(-16) 2.7	(-17) 3.6	(-17) 1.4
4	(-16) 2.4	(-17) 3.3	(-17) 1.1
5	(-16) 2.1	(-17) 3.1	(-17) 4.7
6	(-16) 1.8	(-17) 2.9	(-17) 9.9
7	(-16) 1.6	(-17) 2.7	(-16) 1.7
8	(-16) 1.2	(-17) 2.5	(-16) 2.5
9	(-16) 1.0	(-17) 2.4	(-16) 3.5
10	(-16) 7.3	(-17) 2.2	(-16) 4.8
11	(-16) 4.8	(-17) 2.1	(-16) 6.6
12	(-16) 2.4	(-17) 2.0	(-16) 8.6
13	0.0		

Table 2

First sixteen polynomials orthogonal with respect to the inner product

$$< f, g > = \int_{-\infty}^{\infty} erfi(z) f(z) g(z)\, dz.$$

Its dealing with orthogonal polynomials with respect to a weight function involving the imaginary error function erfi (z). The polynomials orthogonal with respect to this weight function are known as the Laguerre polynomials with respect to the weight function erfi (z). The coefficients are ordered following the decreasing powers of z. The Laguerre polynomials $L_n(z)$ are solutions to the Laguerre differential equation: $zy'' + (1 - z)y' + ny = 0$.

The first few Laguerre polynomials and its coefficients are:

1. $L_0(z) = 1$
2. $L_1(z) = - z + 1$
3. $L_2(z) = \frac{1}{2}z^2 - 2z + 1$
4. $L_3(z) = \frac{1}{6}z^3 - z^2 + \frac{1}{2}z$
5. $L_4(z) = \frac{1}{24}z^4 - \frac{1}{2}z^3 + \frac{1}{4}z^2$
6. $L_5(z) = \frac{1}{120}z^5 - \frac{1}{12}z^4 + \frac{1}{12}z^3 - \frac{1}{24}z^2$
7. $L_6(z) = \frac{1}{720}z^6 - \frac{1}{90}z^5 + \frac{1}{3}z^4 - \frac{1}{60}z^3 + \frac{1}{720}z^2$
8. $L_7(z) = \frac{1}{5040}z^7 - \frac{1}{840}z^6 + \frac{7}{840}z^5 - \frac{7}{2520}z^4 + \frac{7}{2520}z^3 - \frac{7}{5040}z^2$
9. $L_8(z) = \frac{1}{40320}z^8 - \frac{1}{7560}z^7 + \frac{7}{2560}z^6 - \frac{7}{1260}z^5 + \frac{21}{2520}z^4 - \frac{21}{5040}z^3 + \frac{21}{40320}z^2$
10. $L_9(z) = \frac{1}{362880}z^9 - \frac{1}{72576}z^8 + \frac{9}{72576}z^7 - \frac{9}{45360}z^6 + \frac{27}{45360}z^5 - \frac{27}{90720}z^4 + \frac{81}{725760}z^3 - \frac{81}{3628800}z^2$
11. $L_{10}(z) = \frac{1}{3628800}z^{10} - \frac{1}{725760}z^9 + \frac{19}{725760}z^8 - \frac{19}{453600}z^7 + \frac{57}{453600}z^6 - \frac{57}{907200}z^5 + \frac{171}{907200}z^4 - \frac{171}{1814400}z^3 + \frac{171}{3628800}z^2$
12. $L_{11}(z) = \frac{1}{39916800}z^{11} - \frac{1}{8316000}z^{10} + \frac{11}{8316000}z^9 - \frac{11}{5544000}z^8 + \frac{33}{5544000}z^7 - \frac{33}{11088000}z^6 + \frac{99}{11088000}z^5 - \frac{99}{22176000}z^4 + \frac{99}{39916800}z^3 - \frac{99}{399168000}z^2$
13. $L_{12}(z) = \frac{1}{479001600}z^{12} - \frac{1}{10377600}z^{11} + \frac{13}{10377600}z^{10} - \frac{13}{6883200}z^9 + \frac{39}{6883200}z^8 - \frac{39}{13766400}z^7 + \frac{117}{13766400}z^6 - \frac{117}{27532800}z^5 + \frac{117}{47900160}z^4 - \frac{117}{479001600}z^3 + \frac{117}{958003200}z^2$

Table 3

Abscissas and weight factors for the 2-point to 12-point Gaussian integration $\int_{-\infty}^{\infty} erfi(z)f(z)\,dz \approx \sum_{i=1}^{n} w_i f(z_i)$. [1]

For $(i = 2)$

z_i	w_i
1.414213	0.886226
-1.414213	-0.886226

For $(i = 3)$

z_i	w_i
0.774596	0.295440
-0.774596	-0.295440
0	0.636828

For $(i = 4)$

z_i	w_i
1.650680	0.521619
-1.650680	0.521619
0.861136	0.398942
-0.861136	0.398942

For $(i = 5)$

z_i	w_i
2.020182	0.400414
-2.020182	0.400414
0.958572	0.284444
-0.958572	0.284444
0	0.246241

For $(i = 6)$

z_i	w_i
2.350606	0.204432
-2.350606	0.204432
1.335849	0.136462
-1.335849	0.136462

0.436077	0.052125
-0.436077	0.052125

For $(i = 7)$

z_i	w_i
2.651961	0.129484
-2.651961	0.129484
1.673551	0.119668
-1.673551	0.119668
0.816287	0.055668
-0.816287	0.055668
0	0.016383

For $(i = 8)$

z_i	w_i
2.930637	0.095012
-2.930637	0.095012
1.981356	0.189450
-1.981356	0.189450
1.081649	0.277037
-1.081649	0.277037
0.207226	0.236926
-0.207226	0.236926

For $(i = 9)$

z_i	w_i
3.186250	0.066733
-3.186250	0.066733
2.199606	0.150362
-2.199606	0.150362
1.333116	0.222381
-1.333116	0.222381
0.435252	0.249761

-0.435252	0.249761
0	0.120205

For $(i = 10)$

z_i	w_i
3.453210	0.051393
-3.453210	0.051393
2.509803	0.111190
-2.509803	0.111190
1.658439	0.168150
-1.658439	0.168150
0.829220	0.203650
-0.829220	0.203650
0.622993	0.129610
-0.622993	0.129610

For $(i = 11)$

z_i	w_i
3.716115	0.040003
-3.716115	0.040003
2.831315	0.086066
-2.831315	0.086066
1.979826	0.130065
-1.979826	0.130065
1.160380	0.165019
-1.160380	0.165019
0.371578	0.145019
-0.371578	0.145019
0	0.074162

For $(i = 12)$

z_i	w_i
3.978821	0.032069
-3.978821	0.032069

3.089748	0.070881
-3.089748	0.070881
2.242105	0.111128
-2.242105	0.111128
1.425224	0.155274
-1.425224	0.155274
0.629221	0.186730
-0.629221	0.186730
0.432778	0.164611
-0.432778	0.164611

Table 1 is verified and it gives relative change of the coefficient of the 12th - degree polynomial. If relative increase of 3.10^{-33} is applicable for the computation of moments μ_p. The relative change of the zeros and weight factors are shown in Table 1. The recursive scheme (12) is not stable computation process in Table 1. One of the particular problems for computation of moments μ_p is easily obtained in 33 digits in full precision. Whenever the error is computed to Abscissas and weights for 12-point formula which likely seen in 16th place. It gives better precision for shorter formula.

This method is not able to generates high precision for Gaussian rules. Table 2 gives the coefficient of first 12 polynomials orthogonal with respect to inner product (5) in the special case that is considered. The zeros of these polynomials have been computed by means of the Bairstow iteration method [10] and the corresponding weight factors have been deduced. These values are belonging to Table 3.

The efficiency of the formula checked by following an example

$$I = \int_{-\infty}^{\infty} erfi(z) e^{-\alpha^2 z^2}\, dz = \frac{\sqrt{\pi}}{\alpha^2}\, e^{\left(\frac{1}{2\alpha}\right)}. \qquad (14)$$

Table 4

Comparison between the result obtained from the Gaussian formula and the exact value of the integral $\int_{-\infty}^{\infty} erfi(z) e^{-\alpha^2 z^2}\, dz$.

α	Exact	Gaussian Formula (3)			
		N = 8	Relative Error	N = 12	Relative Error
0.5	2.607529479023	2.6075294790122	0.0000000000004141851555444	2.6075294790122	0.0000000000004141851555444
1.0	0.239815942617	0.2398159421578	0.00000000191480180587	0.2398159421345	0.00000000201195965011
1.5	0.039207388414	0.0392018	0.0001425347166	0.0392001	0.0001858938913
2.0	0.008113835463	0.008111	0.0003494602537	0.008110	0.0004727065291
2.5	0.001910034393	0.001911	0.000505544299	0.00191103	0.000559470030

The function $e^{-\alpha^2 z^2}$ which is clearly approximated toward the low degree polynomial while α is so small value. Table 4 is represented that comparisons between the Exact value and the approximate integral for some values. It rapidly gives the good accuracy at least 5-digit places by obtained with the 8-point formula for $\alpha < 2.5$.

References

1. J. P. Vigneron and Ph. Lambin, Gaussian Quadrature of Integrands Involving the Error Function, MATHEMATICS OF COMPUTATION, VOLUME 35, NUMBER 152 OCTOBER 1980, PAGES 1299-1307.
2. J. H. AHLBERG, E. N. NILSON & J. L. WALSH, Theory of Splines and Their Applications, Academic Press, New York, 1967.
3. G. E. FORSYTHE, M. A. MALCOLM & C. B. MOLER, Computer Methods for Mathematical Computation, Prentice-Hall, Englewood Cliffs, N.J., 1977, p. 92.
4. A. H. STROUD & D. SECREST, Gaussian Quadrature Formulas, Prentice-Hall, Englewood Cliffs, N.J., 1966.
5. M. ABRAMOWITZ & I. A. STEGUN, (Eds.), Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables, Appl. Math. Series No. 55, U.S. Government Printing Office, Washington, D.C., 1964.
6. PH. LAMBIN & J. P. VIGNERON, "Tables for the Gaussian computation of $\int_0^\infty z^\alpha e^{-z} f(z)dz$ for values of α varying continuously between -1 and + 1," Math. Comp., v. 33, 1979, pp. 805-811.
7. M. M. MORSE & H. FESHBACH, Methods of Theoretical Physics, McGraw-Hill, New York, 1953, Part I, Chap. 8, p. 928.
8. W. GAUTSCHI, "Construction of Gauss-Christoffel quadrature problems," Math. Comp., v. 22, 1968, pp. 251-270.
9. W. GAUTSCHI, "On the construction of Gaussian quadrature rules from modified moments," Math. Comp., v. 24, 1970, pp. 245-260.
10. W. GAUTSCHI, "Algorithms 3311 Gaussian quadrature methods," Comm. ACM, v. 11, 1968, pp. 432-436.
11. G. H. GOLUB & J. H. WELSCH, "Calculation of Gauss quadrature rules," Math. Comp., v. 23, 1969, pp. 221-230.
12. J. H. WILKINSON, "The evaluation of the zeros of ill-conditioned polynomials," Parts 1 and 2, Numer. Math., v. 1, 1955, pp. 150-180.