MATHEMATICS OF COMPUTATION, VOLUME 35, NUMBER 152
OCTOBER 1980, PAGES 1299–1307

Gaussian Quadrature of Integrands Involving the Error Function

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Abstract. Orthogonal polynomials corresponding to the weight function $1 - \mathrm{erf}(x)$ and defined on the positive real axis are constructed. Abscissas and weight factors for the associated Gaussian quadrature are then deduced (up to 12-point formulas). The stability of the algorithm used for this particular computation is discussed. An example is provided to test the efficiency of the new Gaussian rule.

1. Introduction. In recent years, the field of automatic quadrature has achieved important progress. For tabulated functions with arbitrary grid spacing, cubic spline integrators supply an efficient way to obtain an approximation to a definite integral [1]. In the case where very little is known about the integrand, adaptive quadrature methods [2] can be used with a high probability of success. When possible, however, Gaussian formulas [3] remain extremely interesting, regarding the few integrand evaluations needed. This advantage is especially desirable when the integrand computation is very time consuming. Rather few weight functions and intervals of integration have been considered so far [3]–[5]. In the present paper, a Gaussian quadrature formula is derived for computing expressions of the form

$$I = \int_0^\infty \mathrm{erfc}(x) f(x)\, dx, \tag{1}$$

where

$$\mathrm{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt \tag{2}$$

is the complementary error function [4], and $f(x)$ is a regular function.

To determine the abscissas x_i and weight factors w_i appearing in the Gaussian expression

$$I \approx \sum_{i=1}^{n} w_i f(x_i), \tag{3}$$

it is necessary to obtain the set of orthogonal polynomials $p_k(x)$, $k = 0, 1, \ldots, n$, corresponding to the following scalar product

$$(f, g) = \int_0^\infty \mathrm{erfc}(x) f(x) g(x)\, dx. \tag{4}$$

Received July 25, 1979.
1980 *Mathematics Subject Classification.* Primary 65A05.

The construction of these polynomials and the derivation of the integration formula is treated in Section 2.

2. Orthogonal Polynomials and Gaussian Formula. The Schmidt orthogonalization procedure can be used to generate these polynomials from the set of nonorthogonal functions

$$1, x, x^2, x^3, \dots, x^n. \tag{5}$$

This procedure is described in [6] and amounts to determining recursively the polynomials $p_k(x)$ through the following relation

$$p_0(x) = 1, \tag{6}$$

$$p_k(x) = x^k - \sum_{n=0}^{k-1} \frac{\int_0^\infty \operatorname{erfc}(t) t^k p_n(t) dt}{\int_0^\infty \operatorname{erfc}(t) [p_n(t)]^2 dt} p_n(x), \tag{7}$$

for $k = 1, 2, \dots, n$.

If the explicit expression for these polynomials

$$p_k(x) = \sum_{j=0}^{k} p_j^k x^j \tag{8}$$

is introduced in (6) and (7), the following relation is obtained

$$\sum_{n=0}^{k} p_n^k x^k = x^k - \sum_{n=0}^{k-1} \frac{\sum_{i=0}^n p_i^n \mu_{i+k}}{\sum_{l=0}^n \sum_{i=0}^n p_i^n p_l^n \mu_{i+l}} \sum_{j=0}^{n} p_j^n x^j, \tag{9}$$

where the quantities μ_p are the moments of the weight function

$$\mu_p = \int_0^\infty \operatorname{erfc}(x) x^p \, dx = \frac{\Gamma(p/2 + 1)}{\sqrt{\pi}(p + 1)} . \tag{10}$$

In Eq. (9), the right-hand side can be put under an explicit polynomial form, by reordering the summation on n and j. This leads to the following recursion relations for computing the coefficients p_j^k of the orthogonal polynomials

$$p_k^k = 1, \tag{11}$$

and, for $n \neq k$,

$$p_n^k = -\sum_{j=n}^{k-1} \frac{\sum_{i=0}^j p_i^j \mu_{i+k}}{\sum_{i=0}^j \sum_{l=0}^j p_i^j p_l^j \mu_{i+l}} p_n^j. \tag{12}$$

3. Discussion. A large amount of comments exists in literature on the ill-conditioned character of the problem of determining the zeros and weights for Gaussian rules [7]–[10]. It is not obvious, in a general case, to forecast the stability of relation (12). This question has in fact two different aspects. If one considers the moments μ_k as exactly known quantities, the recursion scheme can propagate the truncation error that affects the coefficients p_j^k at each stage of the recursive process. On the other hand, the polynomial coefficients may be sensitive to errors introduced in computing the moments μ_p. Both effects act to progressively reduce the accuracy of the computed coefficients. Furthermore, the evaluation of the zeros of the polynomials and the subsequent computation of the weight factors will introduce further errors. 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 the 12th-degree orthogonal polynomial coefficients to a slight variation of the moments μ_p. A relative increase of 3.10^{-33} of all moments has been performed. $\Delta p_{12}^i/p_{12}^i$ is the relative change of the polynomial coefficients, $\Delta x_i/x_i$ is the relative change of its zeros, and $\Delta w_i/w_i$ the corresponding relative change in the weight factor.

i	$\left\lvert \frac{\Delta p_{12}^i}{p_{12}^i} \right\rvert$	$\left\lvert \frac{\Delta x_i}{x_i} \right\rvert$	$\left\lvert \frac{\Delta w_i}{w_i} \right\rvert$
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	(-17) 7.3	(-17) 2.2	(-16) 4.8
11	(-17) 4.8	(-17) 2.1	(-16) 6.6
12	(-17) 2.4	(-17) 2.0	(-16) 8.6
13	0.0		

TABLE 2

First sixteen polynomials orthogonal with respect to the scalar product $(f, g) = \int_0^\infty \operatorname{erfc}(x) f(x) g(x)\, dx$. The coefficients are ordered following the decreasing powers of x. For example, the second-degree polynomial is approximately $p_2(x) = x^2 - 1.35x + 0.264$.

```
degree  0

      1.00000 00000 00000

degree  1

(-1)-4.43113 46272 63790
      1.00000 00000 00000

degree  2

(-1) 2.63907 45846 91510
    -1.34782 81344 19103
     1.00000 00000 00000

degree  3

(-1)-1.90171 23800 42575
     1.60432 84210 02063
    -2.55919 01430 63285
     1.00000 00000 00000

degree  4

(-1) 1.57384 90122 88715
    -1.91636 80353 98978
     4.87950 48762 39656
    -4.01618 14460 37398
     1.00000 00000 00000

degree  5

(-1)-1.45181 12915 76531
     2.36388 84058 09562
    -8.47579 47416 00099
 (1) 1.09608 53386 21661
    -5.68398 20904 56470
     1.00000 00000 00000

degree  6

(-1) 1.46418 52508 81862
    -3.03400 78209 90483
 (1) 1.42776 47509 63747
 (1)-2.56745 06962 56243
 (1) 2.07253 25849 80429
    -7.53930 25678 37419
     1.00000 00000 00000

degree  7

(-1)-1.59280 57293 12968
     4.05662 89966 23660
 (1)-2.39403 18949 32827
 (1) 5.59214 87631 00272
 (1)-6.22839 73346 99218
 (1) 3.50528 71260 54658
    -9.56516 01678 28539
     1.00000 00000 00000

degree  8

(-1) 1.85050 52867 50136
    -5.64460 02821 45842
 (1) 4.04596 33619 27969
 (2)-1.17503 25457 81872
 (2) 1.68875 47149 73991
 (2)-1.30437 09256 21547
 (1) 5.48253 01848 02072
 (1)-1.17484 67323 09489
     1.00000 00000 00000

degree  9

(-1)-2.27856 44262 46158
     8.15920 09750 53598
 (1)-6.93607 45469 76045
 (2) 2.42876 44333 11118
 (2)-4.31508 05870 25540
 (2) 4.28075 72282 38953
 (2)-2.45982 69604 81033
 (1) 8.09256 91094 27278
 (1)-1.40787 40810 91919
     1.00000 00000 00000

degree 10

(-1) 2.95562 02971 09199
 (1)-1.22276 58537 98924
 (2) 1.21022 50265 56238
 (2)-4.99433 98195 12650
 (3) 1.06450 41977 91601
 (3)-1.30010 77830 84340
 (2) 9.56226 19830 23607
 (2)-4.28809 32823 86113
 (2) 1.14238 01788 47078
 (1)-1.65473 39858 57488
     1.00000 00000 00000
```

TABLE 2 (*continued*)

degree 11	degree 12
(-1)-4.01902 15677 85816	(-1) 5.70573 59772 00071
(1) 1.89609 50515 51237	(1)-3.03656 33418 48806
(2)-2.15292 50464 52882	(2) 3.90795 17623 25917
(3) 1.02876 29396 70655	(3)-2.13200 37901 17855
(3)-2.57278 58022 54351	(3) 6.14953 08660 11039
(3) 3.75586 15079 64427	(4)-1.04987 70018 11033
(3)-3.39034 95535 63455	(4) 1.12961 43871 16176
(3) 1.94082 76197 81112	(3)-7.91723 32167 89054
(2)-7.03145 11053 27266	(3) 3.65382 64468 93299
(2) 1.55646 93976 48508	(3)-1.09783 83048 90957
(1)-1.91469 83574 97391	(2) 2.06037 64014 77419
1.00000 00000 00000	(1)-2.18714 28498 95518
	1.00000 00000 00000

TABLE 3

Abscissas and weight factors for the 2-point to 12-point Gaussian integration of $\int_0^\infty \operatorname{erfc}(x) f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$.

2-point formula

x_i	w_i
(-1) 2.37734 38919 5	(-1) 4.31362 74656 8
1.11009 37452 2	(-1) 1.32826 83697 3

3-point formula

x_i	w_i
(-1) 1.54164 78808 7	(-1) 3.18951 01760 6
(-1) 7.41558 72890 8	(-1) 2.24661 47274 2
1.66346 66260 7	(-2) 2.05770 93199 8

4-point formula

x_i	w_i
(-1) 1.10435 23644 6	(-1) 2.43861 10764 2
(-1) 5.44173 73334 6	(-1) 2.52484 36824 2
1.22674 99482 9	(-2) 6.51504 63867 3
2.13482 25279 6	(-3) 2.69364 37970 1

5-point formula

x_i	w_i
(-2) 8.41744 61816 4	(-1) 1.93037 95728 9
(-1) 4.21632 83009 9	(-1) 2.48263 05150 5
(-1) 9.63742 64731 8	(-1) 1.08110 44734 5
1.66474 17939 5	(-2) 1.44584 86503 9
2.54969 03572 7	(-4) 3.19640 90482 3

TABLE 3 (*continued*)

6-point formula

x_i	w_i
(-2) 6.69431 49652 0	(-1) 1.57287 34770 0
(-1) 3.39112 56023 9	(-1) 2.31713 66654 3
(-1) 7.84935 94275 0	(-1) 1.38151 69364 9
1.36357 52199 6	(-2) 3.42845 52679 5
2.06126 69281 1	(-3) 2.71682 53055 5
2.92346 87671 3	(-5) 3.54976 70462 2

7-point formula

x_i	w_i
(-2) 5.49123 05061 0	(-1) 1.31182 57034 8
(-1) 2.80385 45936 9	(-1) 2.11756 76314 2
(-1) 6.55644 77802 3	(-1) 1.55184 07675 1
1.14781 30451 2	(-2) 5.66734 24306 1
1.73629 77397 3	(-3) 8.93478 26639 1
2.42423 12979 4	(-4) 4.54210 81438 1
3.26587 55425 8	(-6) 3.75552 25977 5

8-point formula

x_i	w_i
(-2) 4.61168 15858 0	(-1) 1.11498 80399 6
(-1) 2.36840 20722 2	(-1) 1.92042 52854 2
(-1) 5.58296 24892 3	(-1) 1.62489 71991 7
(-1) 9.84661 14109 2	(-2) 7.71608 17817 4
1.49562 40201 2	(-2) 1.89093 96565 5
2.08349 43372 2	(-3) 2.01837 26775 5
2.76002 10216 3	(-5) 6.95612 94614 4
3.58341 35310 3	(-7) 3.82737 13411 6

9-point formula

x_i	w_i
(-2) 3.94542 34273 95065	(-2) 9.62504 34631 75948
(-1) 2.03501 98233 97209	(-1) 1.73913 52569 73502
(-1) 4.82772 14616 51686	(-1) 1.63368 15056 63357
(-1) 8.57033 87015 59237	(-2) 9.36339 79723 28827
1.30815 76394 50268	(-2) 3.12025 34366 38391
1.82534 42453 62237	(-3) 5.40257 21407 42783
2.40835 42904 71411	(-4) 4.08403 26025 89112
3.07346 65214 18331	(-6) 9.94530 47663 76975
3.88065 58812 82185	(-8) 3.78568 70502 76278

10-point formula

x_i	w_i
(-2) 3.42628 01138 86749	(-2) 8.41668 63665 35992
(-1) 1.77312 18994 41196	(-1) 1.57737 80598 10978
(-1) 4.22781 07835 69875	(-1) 1.60300 15054 20744
(-1) 7.54733 44456 28952	(-1) 1.05673 96969 32892
1.15757 30911 38683	(-2) 4.41063 95402 82426
1.62004 57105 40419	(-2) 1.07617 84774 27428
2.13749 28265 08512	(-3) 1.36559 15712 75019
2.71396 59924 26909	(-5) 7.56732 98220 39683
3.36822 21668 40246	(-6) 1.34496 57738 44262
4.16095 05571 17240	(-9) 3.65356 71368 48986

TABLE 3 (*continued*)

11-point formula

	x_i		w_i
(-2)	3.01235 67809 91510	(-2)	7.44055 09878 89769
(-1)	1.56296 82886 65323	(-1)	1.43487 70531 10929
(-1)	3.74198 70530 56710	(-1)	1.54963 63216 15209
(-1)	6.71167 50305 64438	(-1)	1.13709 41476 46168
	1.03398 56465 21831	(-2)	5.62965 55142 88725
	1.45196 45969 91976	(-2)	1.77366 27598 88245
	1.91877 38247 88675	(-3)	3.26453 10661 40002
	2.43357 98552 23858	(-4)	3.12389 65808 86007
	3.00296 80277 35909	(-5)	1.30439 25358 55835
	3.64709 52982 26328	(-7)	1.73694 86390 16921
	4.42682 97204 46769	(-10)	3.45407 07142 18236

12-point formula

	x_i		w_i
(-2)	2.67596 38529 66870	(-2)	6.63896 49104 55207
(-1)	1.39130 82411 60834	(-1)	1.30989 46211 29896
(-1)	3.34211 81025 64531	(-1)	1.48437 89982 53906
(-1)	6.01843 95516 62340	(-1)	1.18464 93278 90080
(-1)	9.30884 38305 86750	(-2)	6.69879 22078 42853
	1.31158 64866 34759	(-2)	2.56988 20629 53840
	1.73714 04275 97650	(-3)	6.26273 84099 13355
	2.20451 49081 77997	(-4)	8.90261 21073 45358
	2.71527 22992 95223	(-5)	6.57595 07884 67420
	3.27754 09264 30984	(-6)	2.11627 18607 02677
	3.91228 24599 57907	(-8)	2.15753 71144 04678
	4.68026 03797 33544	(-11)	3.20845 69902 36600

This check is summarized in Table 1. It gives the relative change of the coefficients of the 12th-degree polynomial when a relative increase of 3.10^{-33} is applied to the moments μ_p used in the computation. The relative change of the zeros and weights is also displayed. This table shows that the recursion scheme (12) is not a stable computation process. However, since a full precision of about 33 digits can be easily obtained in computing the moments μ_p for this particular problem, an error is likely to appear in the 16th place of the computed abscissas and weights for the 12-point formula. For shorter formulas, a better precision is reached.

Though quite general from an algebraic point of view, the method just described is then not obviously applicable to generate high-precision Gaussian rules. For the special case considered here, Table 2 gives the coefficients of the first 12 polynomials orthogonal with respect to the scalar product (4).

The zeros of these polynomials have been computed by means of the Bairstow iteration method [11] and the corresponding weight factors have been deduced. These values are reported in Table 3.

The efficiency of the formula can be checked on the following example

$$I_1 = \int_0^\infty \operatorname{erfc}(x) e^{-\alpha^2 x^2}\, dx = \frac{\operatorname{arctg} \alpha}{\alpha\sqrt{\pi}}\,. \tag{13}$$

TABLE 4
Comparison between the result obtained from the Gaussian formula and the exact value of the integral $\int_0^\infty \operatorname{erfc}(x) e^{-\alpha^2 x^2} dx$.

α	Exact	Gaussian formula (3)			
		n = 8	Relative Error	n = 12	Relative Error
0.5	0.52317 03028 70155 5	0.52317 03028 7025	(−13) 2.	0.52317 03028 70155 5	(−18) 8.
1.0	0.44311 34627 26379 0	0.44311 34616	(−9) 2.	0.44311 34627 24	(−12) 5.
1.5	0.36965 46542 88	0.36965 53	(−6) 2.	0.36965 4657	(−9) 8.
2.0	0.31232 0887	0.31230	(−5) 6.	0.31232 07	(−7) 3.
2.5	0.26861 968	0.26862 0	(−5) 2.	0.26862 0	(−6) 4.

The function $\exp(-\alpha^2 x^2)$ is easily approximated by a low-degree polynomial, especially when α is small. Table 4 gives some points of comparison between the exact and the approximate integral. It can be seen that a good accuracy (at least 5 places) is readily obtained with the 8-point formula for α less than 2.5.

Acknowledgments. The authors are very grateful to the Belgian Fonds National de la Recherche Scientifique for financial support.

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