AN APPROXIMATE FORMULA FOR MULTIPLE INTEGRALS

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Abstract. A fifth degree approximate integration formula for hypercubes is constructed. If the integrand is a real function of n independent real variables and the integer number k satisfying the condition $1 \le k < n$ is given, then a $2^n + \binom{n}{k}2^k + 1$ point non-product quadrature is obtained. In the case n = 4, some comparative numerical examples are considered.

1. Introduction

Here we consider an approximate evaluation to the multiple definite integral

(1.1)
$$I_n^a(f) = \int_{-a}^a \cdots \int_{-a}^a f(x_1, \dots, x_n) \, dx_1 \dots dx_n \,, \quad a > 0 \,.$$

If k is an integer satifying $1 \le k < n$, then a $2^n + {n \choose k} 2^k + 1$ point nonproduct quadrature rule of 5th degree is obtained. The evaluation points of the integrated function f are symmetrically placed over the domain $S_n =$ $[-a, a]^n$ of the integral $I_n^a(f)$. As such the rule is required to be exact for the monomials of degree 0, 2, 4. The constructed approximate integration formula extends the $2^n + 2n + 1$ point quadrature given by Mustard, Lyness and Blatt [2] (see also Stroud [3, p. 233]), and respectively $2^n + n 2^{n-1} + 1$ point quadrature obtained by Das and Pradhan [1].

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2. Fifth Degree Integration Formula

Let us take the following $N = 2^n + \binom{n}{k}2^k + 1$ points: $(\beta_1, \ldots, \beta_n)$, $(\gamma_1, \ldots, \gamma_n)$ and $(0, \ldots, 0)$, where each β_i $(1 \le i \le n)$ is either -a or a, i.e. the corners of the hypercube S_n , k of γ_i $(1 \le i \le n)$ are either $-\alpha a$ or αa and the other ones n - k of γ_i equal to zero. On the one hand we have that the number of $(\beta_1, \ldots, \beta_n)$ type points is 2^n , on the other hand the number of $(\gamma_1, \ldots, \gamma_n)$ type points is $\binom{n}{k}2^k$, and the last type points belong to the (n - k)-faces of the hypercube S_n when the parameter $\alpha \in (0, 1)$. Taking into account that the center of the hypercube S_n is also considered it results that $N = 2^n + \binom{n}{k}2^k + 1$.

We shall construct an approximate rule to $I_n^a(f)$ of the following type

(2.1)
$$Q_{n,k}^{a}(f) = A_0 f(0,...,0) + \sum_{1} f(\gamma_1,...,\gamma_n) + \sum_{2} f(\beta_1,...,\beta_n)$$
.

As we have seen, in the formula (2.1) the the first sum, \sum_{1} , has $\binom{n}{k}2^{k}$ terms, and the second sum, \sum_{2} , has 2^{n} terms. Such that the quadrature (2.1) will be a $2^{n} + \binom{n}{k}2^{k} + 1$ point non-product formula.

The coefficients A_0 , A_1 , A_2 and the parameter α will be determined such as to make the rule exact for all monomials of degree less or equal to five, i.e.

for

(2.3)
$$f = x_1^{k_1} \dots x_n^{k_n}, \quad 0 \le k_1 + \dots + k_n \le 5.$$

We remark the exactness of the formula (2.2) for all monomials (2.3) containing at least one odd power k_i . On the other hand, taking into account that the formula (2.1) has the evaluation points of the function f symmetrically situated over the integration domain S_n (if $\alpha \in (0,1)$), we have to require that (2.2) to be exact only for the monomials

(2.4)
$$f = 1, x_1^2, x_1^4, x_1^2 x_2^2,$$

to obtain a fifth degree exactness quadrature formula.

The exactness conditions of the formula (2.2) for the monomials (2.4) give the following nonlinear algebraic system in A_0 , A_1 , A_2 and α :

(2.5)
$$A_{0} + \binom{n}{k} 2^{k} A_{1} + 2^{n} A_{2} = 2^{n} a^{n},$$
$$2^{k} \binom{n-1}{k-1} a^{2} \alpha^{2} A_{1} + 2^{n} a^{2} A_{2} = 2^{n} \frac{a^{n+2}}{3},$$
$$2^{k} \binom{n-1}{k-1} a^{4} \alpha^{4} A_{1} + 2^{n} a^{4} A_{2} = 2^{n} \frac{a^{n+4}}{5},$$
$$2^{k} \binom{n-2}{k-2} a^{4} \alpha^{4} A_{1} + 2^{n} a^{4} A_{2} = 2^{n} \frac{a^{n+4}}{9},$$

or equivalently

(2.6)
$$A_{0} + \binom{n}{k} 2^{k} A_{1} + 2^{n} A_{2} = 2^{n} a^{n},$$
$$2^{k} \binom{n-1}{k-1} \alpha^{2} A_{1} + 2^{n} A_{2} = 2^{n} \frac{a^{n}}{3},$$
$$2^{k} \binom{n-1}{k-1} \alpha^{4} A_{1} + 2^{n} A_{2} = 2^{n} \frac{a^{n}}{5},$$
$$2^{k} \binom{n-2}{k-2} \alpha^{4} A_{1} + 2^{n} A_{2} = 2^{n} \frac{a^{n}}{9}.$$

Using the third and fourth equations of (2.6) we get the coefficient

(2.7)
$$A_2 = \frac{5n - 9k + 4}{45(n-k)}a^n.$$

Then from the second and third equations of (2.6) we obtain

(2.8)
$$\alpha^2 = \frac{2(n-1)}{5n-3k-2}, \qquad A_1 = \frac{2^{n-k}(5n-3k-2)^2}{45(n-1)(n-k)\binom{n-1}{k-1}}a^n.$$

Finally, from the first equation of (2.6) we get

(2.9)
$$A_0 = -\frac{2^n \left[25n^2 - 5\left(9k+4\right)n + 4\left(9k+1\right)\right]}{45k \left(n-1\right)} a^n$$

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Thus we have obtained the following quadrature rule

$$(2.10) \qquad Q_{n,k}^{a}(f) \\ = \frac{a^{n}}{45} \left[-\frac{2^{n} \left[25n^{2} - 5\left(9k + 4\right)n + 4\left(9k + 1\right) \right]}{k\left(n - 1\right)} f\left(0, \dots, 0\right) \right. \\ \left. + \frac{2^{n-k} \left(5n - 3k - 2\right)^{2}}{\left(n - 1\right)\left(n - k\right) \binom{n-1}{k-1}} \sum_{1} f\left(\gamma_{1}, \dots, \gamma_{n}\right) \right. \\ \left. + \frac{5n - 9k + 4}{\left(n - k\right)} \sum_{2} f\left(\beta_{1}, \dots, \beta_{n}\right) \right].$$

We remark that for k fulfiling $1 \le k < n$ the parameter α satisfies $\alpha^2 < 1$, such that the $(\gamma_1, \ldots, \gamma_n)$ type points are placed over the domain S_n .

It will be interesting to obtain the quadrature formula (2.10) which has all the coefficients positive. In the next section we shall give such a quadrature formula.

3. Particular Cases

1. Mustard-Lyness-Blatt quadrature formula [2; 4, p. 233]. This quadrature is obtained considering k = 1. In this case from the (2.8), (2.9), (2.7) we get

(3.1)
$$\alpha^{2} = \frac{2}{5} \quad \left(\alpha = \sqrt{\frac{2}{5}}\right),$$
$$A_{0} = \frac{2^{n} (8 - 5n)}{9} a^{n}, \quad A_{1} = \frac{5 \cdot 2^{n-1}}{9} a^{n}, \quad A_{2} = \frac{1}{9} a^{n},$$

and the corresponding quadrature formula is

(3.2)
$$Q_{n,1}^{a}(f) = \frac{a^{n}}{9} \left[2^{n} (8-5n) f(0,\ldots,0) + 5 \cdot 2^{n-1} \sum_{1} f\left(0,\ldots,0,\pm a\sqrt{\frac{2}{5}},0,\ldots,0\right) + \sum_{2} f(\pm a,\ldots,\pm a) \right].$$

Taking into account that all evaluation points of the first sum, \sum_1 , have the coordinates zero excepting one of the coordinates which is either $-a\sqrt{\frac{2}{5}}$

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or $a\sqrt{\frac{2}{5}}$, this sum contains 2n terms, and the second sum, \sum_2 , contains 2^n terms, so it results that (3.2) is a $2^n + 2n + 1$ non-product quadrature of fifth degree.

2. Das-Pradhan quadrature formula [1]. This quadrature is obtained considering k = n - 1. In this case from the (2.8), (2.9), (2.7) we get

(3.3)
$$\alpha^{2} = \frac{2(n-1)}{2n+1},$$
$$A_{0} = \frac{2^{n} (20n^{2} - 61n + 32)}{45(n-1)^{2}} a^{n}, \quad A_{1} = \frac{2(2n+1)^{2}}{45(n-1)^{2}} a^{n},$$
$$A_{2} = \frac{13 - 4n}{45} a^{n},$$

and the corresponding quadrature formula is

$$(3.4) \quad Q_{n,n-1}^{a}(f) = \frac{a^{n}}{45} \left[\frac{2^{n} \left(20n^{2} - 61n + 32 \right)}{\left(n-1\right)^{2}} f\left(0, \dots, 0\right) \right. \\ \left. + \frac{2 \left(2n+1\right)^{2}}{\left(n-1\right)^{2}} \sum_{1} f\left(\pm a\alpha, \dots, \pm a\alpha, 0, \pm a\alpha, \dots, \pm a\alpha\right) \right. \\ \left. + \left(13 - 4n\right) \sum_{2} f\left(\pm a, \dots, \pm a\right) \right].$$

Taking into account that all evaluation points of the first sum, \sum_1 , have a coordinate equals to zero and all the other ones are either $-a\alpha$ or $a\alpha$, this sum contains $n 2^{n-1}$ terms, the second sum \sum_2 , contains 2^n terms, so it results that (3.4) is a $2^n + n2^{n-1} + 1$ non-product quadrature of fifth degree.

We remark that the Das-Pradhan quadrature formula, in the case n = 2, for which was derived the asymptotic error estimate in [1], is the same with the Mustard-Lyness-Blatt quadrature formula.

3. Quadrature with positive coefficients. At the begin, we remark that the Mustard–Lyness–Blatt quadrature has not all the coefficients positive. Indeed, the coefficient $A_0 = \frac{2^n(8-5n)}{9}a^n$ is negative for all $n \ge 2$.

Das–Pradhan class quadratures has only one quadrature rule with all the coefficients positive. It is obtained for n = 3. The other ones have a negative coefficient, either

$$A_2 = \frac{13 - 4n}{45}a^n < 0, \quad n \ge 4.$$

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$$A_0 = \frac{2^n \left(20n^2 - 61n + 32\right)}{45 \left(n - 1\right)} a^n < 0, \quad n = 2$$

Because A_1 is always positive, to obtain quadrature rules of the type (2.10) having all the coefficients positive, the following conditions must be satisfied

$$(3.5) 25n^2 - 5(9k+4)n + 4(9k+1) < 0, A_0 > 0,$$

and

$$(3.6) 5n - 9k + 4 > 0, A_2 > 0.$$

Ouside of the above mentioned quadrature with positive coefficients (Das-Pradhan quadrature with n = 3), we give the only one quadrature formula having positive coefficients in the case n = 5, k = 3. It is

(3.7)
$$Q_{5,3}^{a}(f) = \frac{a^{5}}{135} \left[304f(0,\dots,0) + 49 \sum_{1} f(\pm a\alpha, \pm a\alpha, \pm a\alpha, 0, 0) + 3 \sum_{2} f(\pm a, \dots, \pm a) \right],$$

where $\alpha = 2/\sqrt{7}$.

4. Numerical Examples

To compare the quadrature rules obtained by Mustard-Lyness-Blatt, and by Das-Pradhan (the both being particular cases of the quadrature formula (2.10), k = 1 and k = n - 1 respectively) with the new one obtained here, i.e. for k satisfying 1 < k < n - 1, we have considered the three quadratures when n = 4.

The Mustard-Lyness-Blatt quadrature (n = 4, k = 1) has the coefficients

$$A_0 = -\frac{64}{3}a^4$$
, $A_1 = \frac{40}{9}a^4$, $A_2 = \frac{1}{9}a^4$,

and $\alpha^2 = 2/5$.

The new one quadrature (n = 4, k = 2) has the coefficients

$$A_0 = -\frac{32}{15}a^4$$
, $A_1 = \frac{32}{45}a^4$, $A_2 = \frac{1}{15}a^4$,

and $\alpha^2 = 1/2$.

The Das-Pradhan quadrature (n = 4, k = 3) has the coefficients

$$A_0 = \frac{64}{15}a^4$$
, $A_1 = \frac{2}{5}a^4$, $A_2 = -\frac{1}{15}a^4$,

and $\alpha^2 = 2/3$.

In the given table the exact and approximate values and also the error bounds are presented for the following four functions:

$$f(x, y, z, t) = \frac{1}{(5 + x + y + z + t)^4},$$

with

$$I_4^a(f) = \frac{1}{6} \left[4 \log \left(25 - 4a^2 \right) - \log \left(25 - 16a^2 \right) - 6 \log 5 \right];$$
$$f(x, y, z, t) = e^{xyzt},$$

with $I_{4}^{a}\left(f\right)$ computed by series expansions;

$$f(x, y, z, t) = \sqrt{4 + x + y + z + t},$$

with

$$\begin{split} I_4^a\left(f\right) &= \frac{1024}{945} \left[8 \left(1+a\right)^4 \sqrt{1+a} - \left(2+a\right)^4 \sqrt{2+a} \right. \\ &- \left(2-a\right)^4 \sqrt{2-a} + 8 \left(1-a\right)^4 \sqrt{1-a} + 48 \right] \,; \\ &\left. f\left(x,y,z,t\right) = \frac{1}{\sqrt{5+x+y+z+t}} \,, \end{split}$$

with

$$I_4^a(f) = \frac{16}{105} \left[(5+4a)^3 \sqrt{5+4a} - 4 (5+2a)^3 \sqrt{5+2a} - 4 (5-2a)^3 \sqrt{5-2a} + (5-4a)^3 \sqrt{5-4a} + 750\sqrt{5} \right]$$

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а	$I_4^a(f)$	$Q^a_{4,1}(f)$	Err	$Q^a_{4,2}(f)$	Err	$Q^a_{4,2}(f)$	Err
$ \begin{array}{c} 1 \\ 0.5 \\ 0.25 \end{array} $	5.40396E-02	1.50254E-01	9.62E-02	1.09288E-01	5.52E-02	-5.69933E-03	5.97E-02
	1.84423E-03	1.85169E-03	7.45E-06	1.84768E-03	3.45E-06	1.83993E-03	4.30E-06
	1.03442E-04	1.03447E-04	5.08E-09	1.03444E-04	2.19E-09	1.03439E-04	2.79E-09
$\begin{array}{c} 1 \\ 0.5 \\ 0.25 \end{array}$	1.63133E 01	1.69655E 01	6.52E-01	1.65793E 01	2.66E-01	1.54207E 01	8.93E-01
	1.00007E 00	1.00022E 00	1.45E-04	1.00013E 00	5.79E-05	9.99870E-01	2.03E-04
	6.25000E-02	6.25000E-02	3.53E-08	6.25000E-02	1.41E-08	6.25000E-02	4.94E-08
$\begin{array}{c} 1 \\ 0.5 \\ 0.25 \end{array}$	3.16372E 01	3.15853E 01	5.19E-02	3.16077E 01	2.95E-02	3.16688E 01	3.16E-02
	1.99470E 00	1.99469E 00	6.88E-06	1.99469E 00	3.05E-06	1.99407E 00	3.86E-06
	1.24918E-01	1.24918E-01	5.55E-09	1.24918E-01	2.35E-09	1.24918E-01	3.11E-09
$ \begin{array}{c} 1 \\ 0.5 \\ 0.25 \end{array} $	7.31713E 00	7.32778E 00	1.06E-02	7.32255E 00	5.42E-03	7.31070E 00	6.44E-03
	4.49511E-01	4.49515E-01	4.28E-06	4.49513E-01	1.88E-06	4.49509E-01	2.39E-06
	2.79860E-02	2.79869E-02	3.46E-09	2.79860E-02	1.41E-09	2.79860E-02	2.08E-09

The numerical results in the table are given in the order of presented examples.

We remark that for all considered examples the least error values are are obtained in the case k = 2.

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