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Two-dimensional quadrature for functions with a point singularity

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Abstract. Numerical integration over the unit square of functions having a weak singularity at a vertex is considered. The cubature formula resulting from using in both directions a one-dimensional composite quadrature formula on graded grid is studied. The dependence of the error of the cubature rule on nonuniformity of the grid is investigated and the conditions for the grid under which the method has the maximal possible convergence rate are found. Theoretical results are verified by numerical examples in the case of the Gaussian quadrature.

Key words: two-dimensional quadrature, point singularity, graded grid.

1. INTRODUCTION

We consider numerical evaluation of the double integral

$$\int_0^1 \int_0^1 f(x,y)dxdy, \tag{1}$$

where the integrand f is continuous in the unit square

$$G = \{(x,y) : 0 < x < 1, \, 0 < y < 1\}$$

and satisfies the condition

$$\left|f(x,y)\right| \le c_0\left(x^2 + y^2\right)^{-\nu/2}, \quad (x,y) \in G, \tag{2}$$

where $0 < \nu < 2$. Such a function is in general unbounded at the origin $(0,0)$.

If the integration region is a rectangle and the integrand has a weak singularity at its vertex, then we can get with the help of an affine transformation the integral (1). But if the integrand has a weak singularity at a point in the rectangle or on a side of it, then we can divide this region into two or four rectangles so that the integrand has a singularity only at a vertex of each of the new rectangles. It is necessary to compute such integrals, for example, when solving weakly singular integral equations by the collocation method (see, e.g., [1]).

If the integrand function has a singularity, then the convergence of standard quadrature methods may be very poor [2]. The present paper deals with the cubature formulas which we get using in both directions a one-dimensional composite quadrature formula on graded grid [3,4]. We choose the grid points so that a high-order convergence is obtained. The use of such quadrature formulas for the solution of one-dimensional weakly singular integral equations is studied in [5].

Note that in [6,7] the adaptive quadrature for functions with a point singularity is studied. But if the type of the singularity is known, it is better to determine a suitable grid in advance, instead of using an adaptive method.

We shall construct an appropriate cubature formula for the evaluation of the integral (1) in the following way.

We use a one-dimensional quadrature formula

$$\int_{-1}^{1} g(\xi)d\xi \approx \sum_{p=1}^{m} w_p g(\xi_p), \tag{3}$$

which is exact for all polynomials of degree μ, $0 \leq m-1 \leq \mu \leq 2m-1$, for instance, for the trapezoidal rule $m = 2$ and $\mu = 1$, for Simpson's rule $m = 3$ and $\mu = 3$, for Gaussian quadrature $\mu = 2m-1$. We assume that the knots of the formula (3) satisfy the conditions

$$-1 \leq \xi_1 < \xi_2 < \ldots < \xi_m \leq 1 \tag{4}$$

and the weights $w_p > 0$, $p = 1, \ldots, m$. Then

$$\sum_{p=1}^{m} w_p = 2\,. \tag{5}$$

We divide the interval $(0, 1)$ with grid points

$$x_i = \left(\frac{i}{N}\right)^r, \quad i = 0, 1, \ldots, N,$$

into N subintervals (x_{i-1}, x_i), $i = 1, \ldots, N$. Here the real number $r \geq 1$ characterizes the nonuniformity of the grid. If $r = 1$, then the grid points are uniformly located. Using the transformation

$$x = x_{i-1} + \frac{1}{2}(\xi + 1)(x_i - x_{i-1}),$$

we transfer the knots into $[x_{i-1}, x_i]$:

$$\xi_{ip} = x_{i-1} + \frac{1}{2}(\xi_p + 1)(x_i - x_{i-1}), \quad p = 1, \dots, m\,. \tag{6}$$

Then from (3) it follows

$$\int\limits_{x_{i-1}}^{x_i} J(x)dx \approx \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p J(\xi_{ip}), \quad i = 1, \dots, N\,. \tag{7}$$

As in general the integrand $f(x,y)$ is unbounded in the neighbourhood of the origin $(0,0)$, then by constructing the cubature formula we replace it with 0 in the (small) square

$$G_{11} = \{(x,y):\ 0 < x < x_1,\ 0 < y < x_1\}$$

and denote

$$f_N(x,y) = \begin{cases} 0 & \text{if} \quad (x,y) \in G_{11}\,, \\ f(x,y) & \text{if} \quad (x,y) \in G \setminus \overline{G}_{11}\,. \end{cases}$$

The corresponding error

$$Q_N = \int\limits_G [f(x,y) - f_N(x,y)]dxdy = \int\limits_{G_{11}} f(x,y)dxdy\,.$$

We denote

$$J(x) = \int\limits_0^1 f_N(x,y)dy\,. \tag{8}$$

Using the formula (7), we get

$$\begin{aligned} \int\limits_0^1 \int\limits_0^1 f(x,y)dxdy &= \int\limits_0^1 J(x)dx + Q_N \\ &= \sum_{i=1}^{N} \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p J(\xi_{ip}) + Q_N + R_N \\ &= \sum_{i=1}^{N} \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p \sum_{j=1}^{N} \frac{1}{2}(x_j - x_{j-1}) \\ &\quad \times \sum_{q=1}^{m} w_q f_N(\xi_{ip}, \xi_{jq}) + Q_N + R_N + S_N, \end{aligned}$$

where R_n and S_n are the errors of quadrature formulas.

So we get the cubature formula

$$\int_0^1 \int_0^1 f(x,y)dxdy = \sum_{i,j=1}^{N} \frac{1}{4}(x_i - x_{i-1})(x_j - x_{j-1}) \sum_{p,q=1}^{m} w_p w_q f_N(\xi_{ip}, \xi_{jq}) + Q_N + R_N + S_N \,. \tag{9}$$

Here and below, if either $\xi_{i1} = x_{i-1}$ or $\xi_{im} = x_i$, then we define the value of a function at ξ_{i1} or ξ_{im}, respectively, as the limit from the right or from the left. Thus $f_N(\xi_{1p}, \xi_{1q}) = 0$ and $f_N(\xi_{ip}, \xi_{jq}) = f(\xi_{ip}, \xi_{jq})$ if $i > 1$ or $j > 1$.

To estimate the error of the formula (9), we assume that the integrand $f(x,y)$ has in the square G continuous partial derivatives with respect to x and y until the order $\mu + 1$ and satisfies the conditions

$$\begin{aligned} \Big| \frac{\partial^{\mu+1}}{\partial x^{\mu+1}} f(x,y) \Big| &\le c_1 (x^2 + y^2)^{-(\nu+\mu+1)/2}, \\ \Big| \frac{\partial^{\mu+1}}{\partial y^{\mu+1}} f(x,y) \Big| &\le c_2 (x^2 + y^2)^{-(\nu+\mu+1)/2}, \quad (x,y) \in G \,. \end{aligned} \tag{10}$$

We present two examples of the functions which satisfy the conditions (2) and (10). In these examples $h(x,y)$ is a function which has on the closed square $\overline{G}$ continuous partial derivatives with respect to x and y up to the order $\mu + 1$.

1. The function

$$f(x,y) = (\gamma_1 x + \gamma_2 y)^{-\alpha} (\gamma_3 x^2 + \gamma_4 y^2)^{-\beta/2} h(x,y)$$

satisfies the conditions (2) and (10) with $\nu = \alpha + \beta$ if $0 < \alpha + \beta < 2$ and γ_p, $p = 1,2,3,4$, are positive constants.

2. The function

$$f(x,y) = (\gamma_1 x + \gamma_2 y)^{-\alpha} (\gamma_3 x^2 + \gamma_4 y^2)^{-\beta/2} \big[\log(\gamma_5 x^2 + \gamma_6 y^2) \big]^k h(x,y)$$

satisfies the conditions (2) and (10) with $\nu = \alpha + \beta + \varepsilon$ if $0 < \alpha + \beta < 2$, k is a positive integer and γ_p, $p = 1, 2, \dots, 6$, are positive constants. Here ε is an arbitrary (small) positive constant such that $\alpha + \beta + \varepsilon < 2$.

It is well known (see, e.g., [8]) that if integrand $f \in C^{\mu+1}(\overline{G})$ and $f_N(x,y) = f(x,y)$ (then $Q_N = 0$), then the maximal possible convergence rate $R_N + S_N = O(N^{-\mu-1})$ is obtained in the case of a uniform grid ($r = 1$). In the next section we show that the same convergence rate can be achieved also for the integrands satisfying the conditions (2) and (10) if we choose an appropriate graded grid.

2. THE ESTIMATE FOR THE ERROR OF THE CUBATURE FORMULA

For the convergence rate of the cubature formula (9) the following result is valid.

Theorem. *Let the following conditions be fulfilled*

1. *The quadrature formula* (3) *is exact for all polynomials of degree* μ, $0 \leq m-1 \leq \mu \leq 2m-1$, *its weights* $w_p > 0$, $p = 1, \dots, m$, *and its knots satisfy the conditions* (4).

2. *The integrand* $f(x,y)$ *is continuous and has continuous partial derivatives with respect to* x *and* y *up to the order* $\mu+1$ *in the square* G *and in this square the estimates* (2) *and* (10) (*where* $0 < \nu < 2$) *hold.*

3. *In the formula* (9) *grid points* $x_i = (i/N)^r$, $i = 0, 1, \dots, N$, $r \geq 1$, *and knots* ξ_{ip} *are expressed in the form* (6).

Then for the error of the cubature formula (9) *the following estimates hold*:

$$\big|Q_N + R_N + S_N\big| \leq c \begin{cases} N^{-r(2-\nu)} & \textit{if} \quad 1 \leq r < \frac{\mu+1}{2-\nu}, \\ N^{-\mu-1}\ln N & \textit{if} \qquad r = \frac{\mu+1}{2-\nu}, \\ N^{-\mu-1} & \textit{if} \qquad r > \frac{\mu+1}{2-\nu}. \end{cases} \tag{11}$$

Proof. We shall estimate the errors Q_N, R_N, and S_N separately.

Using the conditions (2) and the change of variables

$$x = \varrho\cos\theta, \qquad y = \varrho\sin\theta,$$

we estimate

$$\begin{aligned} \big|Q_N\big| &= \Big|\int_0^{x_1}\int_0^{x_1} f(x,y)dxdy\Big| \leq c_0 \int_0^{x_1}\int_0^{x_1} \big(x^2+y^2\big)^{-\nu/2}dxdy \\ &\leq c_0 \int_0^{\pi/2}\int_0^{x_1\sqrt{2}} \varrho^{-\nu+1}d\varrho d\theta = c_3 x_1^{2-\nu}. \end{aligned}$$

As $x_1 = N^{-r}$, we get

$$\big|Q_N\big| \leq c_3 N^{-r(2-\nu)}\,. \tag{12}$$

To estimate R_N and S_N, we use some ideas from [1,4]. If $\mu > m-1$, then in addition to the knots $\xi_1, \dots, \xi_m$ we fix in the interval $(-1,1)$ additional $\mu-m+1$ knots $\xi_{m+1}, \dots, \xi_{\mu+1}$ so that $\xi_i \neq \xi_j$ if $i \neq j$ and generate by the formula (6) the corresponding knots $\xi_{ip} \in (x_{i-1}, x_i)$, $p = m+1, \dots, \mu+1$, $i = 1, \dots, N$. We define the interpolation projector P_N by the formula

$$\big(P_N J\big)(x) = \sum_{p=1}^{\mu+1} J\big(\xi_{ip}\big)\varphi_{ip}(x), \quad x \in (x_{i-1}, x_i),\ i = 1, \dots, N\,,$$

where

$$\varphi_{ip}(x) = \prod_{\substack{q=1\\q\neq p}}^{\mu+1} \frac{x-\xi_{iq}}{\xi_{ip}-\xi_{iq}}\,.$$

Then $\big(P_N J\big)(x)$ is on every interval (x_{i-1}, x_i), $i = 1, \dots, N$, a polynomial of the degree not exceeding μ,

$$\big(P_N J)(\xi_{ip}) = J(\xi_{ip}), \quad p = 1, \dots, \mu+1,\ i = 1, \dots, N\,,$$

and

$$\sup_{x_{i-1}<x<x_i} \big|\varphi_{ip}(x)\big| = \sup_{-1<\xi<1} \left| \prod_{\substack{q=1\\q\neq p}}^{\mu+1} \frac{\xi-\xi_q}{\xi_p-\xi_q} \right| = d_p$$

does not depend on i and N.

Let $J(x)$ be defined by the formula (8). Due to the exactness of the formula (7) for the polynomials of the degree μ we have

$$R_N = \int_0^1 \big[J(x) - \big(P_N J\big)(x)\big]\,dx\,.$$

Let $v(x)$ be an arbitrary polynomial of the degree not exceeding μ. Then $\big(P_N v\big)(x) = v(x)$ and

$$\begin{aligned}
&\sup_{x_{i-1}<x<x_i} \big|J(x) - \big(P_N J\big)(x)\big| \\
&\qquad \le \sup_{x_{i-1}<x<x_i} \big|J(x) - v(x)\big| + \sup_{x_{i-1}<x<x_i} \big|\big(P_N v\big)(x) - \big(P_N J\big)(x)\big| \\
&\qquad \le \Big(1 + \sum_{p=1}^{\mu+1} d_p\Big) \sup_{x_{i-1}<x<x_i} \big|J(x) - v(x)\big|\,.
\end{aligned}$$

If $v(x)$ is the Taylor polynomial

$$v(x) = \sum_{q=0}^{\mu} \frac{1}{q\,!} J^{(q)}(x_i)(x-x_i)^q, \quad x \in (x_{i-1}, x_i)\,,$$

then

$$J(x) - v(x) = \frac{1}{\mu!} \int_{x_i}^{x} (x-s)^{\mu} J^{(\mu+1)}(s)\,ds, \quad x \in (x_{i-1}, x_i)\,,$$

and therefore

$$\sup_{x_{i-1}<x<x_i} \big|J(x) - \big(P_N J\big)(x)\big| \le c \sup_{x_{i-1}<x<x_i} \Big|\int\limits_{x_i}^{x} (x-s)^{\mu} J^{(\mu+1)}(s)ds\Big|, \quad (13)$$

$$i = 1, \ldots, N\,.$$

By c we denote a constant whose value changes from time to time and which does not depend on i, j, and N.

If $x \in (0, x_1)$, then with the help of (10) we estimate

$$\begin{aligned} \Big|J^{(\mu+1)}(x)\Big| &= \Big|\int\limits_{x_1}^{1} \frac{\partial^{\mu+1}}{\partial x^{\mu+1}} f(x,y)dy\Big| \le c_1 \int\limits_{x_1}^{1} \big(x^2+y^2\big)^{-(\nu+\mu+1)/2} dy \\ &\le c_1 \int\limits_{x_1}^{1} y^{-\nu-\mu-1} dy \le c x_1^{-\nu-\mu}\,. \end{aligned}$$

But if $x \in (x_1, 1)$, then

$$\begin{aligned} \Big|J^{(\mu+1)}(x)\Big| &= \Big|\int\limits_{0}^{1} \frac{\partial^{\mu+1}}{\partial x^{\mu+1}} f(x,y)dy\Big| \le c_1 \int\limits_{0}^{1} \big(x^2+y^2\big)^{-(\nu+\mu+1)/2} dy \\ &\le c_1 \int\limits_{0}^{x} x^{-\nu-\mu-1} dy + c_1 \int\limits_{x}^{1} y^{-\nu-\mu-1} dy \le c x^{-\nu-\mu}\,. \end{aligned}$$

Using in (13) these estimates and the inequality $x_{i-1} \ge 2^r x_i$, $i = 2, \ldots, N$, we get

$$\sup_{x_{i-1}<x<x_i} \big|J(x) - \big(P_N J\big)(x)\big| \le c(x_i - x_{i-1})^{\mu+1} x_i^{-\nu-\mu}\,, \quad i = 1, \ldots, N\,,$$

and therefore

$$\begin{aligned} \big|R_N\big| &= \Big|\sum_{i=1}^{N} \int\limits_{x_{i-1}}^{x_i} \big[J(x) - \big(P_N J\big)(x)\big]dx\Big| \\ &\le c \sum_{i=1}^{N} (x_i - x_{i-1})^{\mu+2} x_i^{-\nu-\mu}\,. \end{aligned}$$

As

$$x_i = \Big(\frac{i}{N}\Big)^r \quad \text{and} \quad 0 < x_i - x_{i-1} \le r\frac{i^{r-1}}{N^r},$$

we get

$$\big|R_N\big| \le cN^{-r(2-\nu)} \sum_{i=1}^{N} i^{r(2-\nu)-\mu-2}$$

and thus

$$\big|R_N\big| \le c \begin{cases} N^{-r(2-\nu)} & \text{if} \quad r(2-\nu) < \mu+1\,, \\ N^{-\mu-1}\ln N & \text{if} \quad r(2-\nu) = \mu+1\,, \\ N^{-\mu-1} & \text{if} \quad r(2-\nu) > \mu+1\,. \end{cases} \tag{14}$$

Now we begin to estimate the error

$$S_N = \sum_{i=1}^{N} \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p \Big[J(\xi_{ip}) - \sum_{j=1}^{N} \frac{1}{2}(x_j - x_{j-1}) \sum_{q=1}^{m} w_q f_N(\xi_{ip}, \xi_{jq}) \Big].$$

If we denote

$$S_{Nj}(\xi_{ip}) = \int\limits_{x_{j-1}}^{x_j} f_N(\xi_{ip}, y)dy - \frac{1}{2}(x_j - x_{j-1}) \sum_{q=1}^{m} w_q f_N(\xi_{ip}, \xi_{jq}),$$

then

$$S_N = \sum_{i=1}^{N} \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p \sum_{j=1}^{N} S_{Nj}(\xi_{ip})\,. \tag{15}$$

As

$$(P_N f_N)(\xi_{ip}, y) = \sum_{q=1}^{\mu+1} f_N(\xi_{ip}, \xi_{jq}) \varphi_{jq}(y)$$

is in the interval $y \in (x_{j-1}, x_j)$, $j = 1, \dots, N$, a polynomial with respect to y of degree not exceeding μ and $(P_N f_N)(\xi_{ip}, \xi_{jq}) = f_N(\xi_{ip}, \xi_{jq})$, we have

$$S_{Nj}(\xi_{ip}) = \int\limits_{x_{j-1}}^{x_j} \Big[f_N(\xi_{ip}, y) - (P_N f_N)(\xi_{ip}, y) \Big] dy\,.$$

As $f_N(x, y) = 0$, $(x, y) \in G_{11}$, we get $S_{N1}(\xi_{1p}) = 0$, $p = 1, \dots, m$. If either $i > 0$ or $j > 1$, then estimating as above gives

$$
\begin{aligned}
\left|S_{Nj}(\xi_{ip})\right| &\le (x_j - x_{j-1}) \sup_{x_{j-1}<y<x_j} \left| f_N(\xi_{ip}, y) - (P_N f_N)(\xi_{ip}, y)\right| \\
&\le c(x_j - x_{j-1}) \sup_{x_{j-1}<y<x_j} \left| \int_{x_j}^{y} (y-s)^{\mu} \frac{\partial^{\mu+1}}{\partial y^{\mu+1}} f(\xi_{ip}, y) dy \right| \\
&\le c\, c_2 (x_j - x_{j-1})^{\mu+2} \big(x_{i-1}^2 + x_{j-1}^2\big)^{-(\nu+\mu+1)/2} .
\end{aligned}
$$

Due to (15) and (5) we get

$$
\begin{aligned}
\left|S_N\right| &= \Bigg| \sum_{i=2}^{N} \Bigg[\sum_{j=1}^{i} \frac{1}{2}(x_i - x_{i-1}) \sum_{p=1}^{m} w_p S_{Nj}(\xi_{ip}) \\
&\quad + \sum_{j=1}^{i-1} \frac{1}{2}(x_j - x_{j-1}) \sum_{p=1}^{m} w_p S_{Ni}(\xi_{jp}) \Bigg] \Bigg| \\
&\le c \sum_{i=2}^{N} \Bigg[\sum_{j=1}^{i} (x_i - x_{i-1})(x_j - x_{j-1})^{\mu+2} \big(x_{i-1}^2 + x_{j-1}^2\big)^{-(\nu+\mu+1)/2} \\
&\quad + \sum_{j=1}^{i-1} (x_j - x_{j-1})(x_i - x_{i-1})^{\mu+2} \big(x_{j-1}^2 + x_{i-1}^2\big)^{-(\nu+\mu+1)/2} \Bigg] \\
&\le 2c \sum_{i=2}^{N} i (x_i - x_{i-1})^{\mu+3} x_{i-1}^{-\nu-\mu-1} .
\end{aligned}
$$

The last inequality is a consequence from the estimates $x_{i-1}^2 + x_{j-1}^2 \ge x_{i-1}^2$ and $x_j - x_{j-1} \le x_i - x_{i-1}$ if $j \le i$. As in estimating R_N, we get here

$$
\left|S_N\right| \le c \begin{cases} N^{-r(2-\nu)} & \text{if} \quad r(2-\nu) < \mu + 1 \,, \\ N^{-\mu-1} \ln N & \text{if} \quad r(2-\nu) = \mu + 1 \,, \\ N^{-\mu-1} & \text{if} \quad r(2-\nu) > \mu + 1 \,. \end{cases}
$$

Together with (12) and (14), the estimates (11) follow.

3. NUMERICAL EXAMPLES

We consider the computation of the integral

$$
\int_0^1 \int_0^1 \sqrt[3]{\frac{x+y}{(x^2+2y^2)^2}}\, dx dy = 1.504\,558\,921\,379\,898.
$$

Table 1. The errors of the cubature formula

N	$r=3$		$r=5$		$r=7$	
	ε_N	ϱ_N	ε_N	ϱ_N	ε_N	ϱ_N
4	2.4 E-2		3.2 E-3		4.5 E-3	
8	3.0 E-3	8.0	1.3 E-4	25.5	1.6 E-4	28.6
16	3.8 E-4	8.0	4.4 E-6	28.8	3.5 E-6	45.4
32	4.7 E-5	8.0	1.4 E-7	30.4	6.4 E-8	54.6
64	5.9 E-6	8.0	4.6 E-9	31.2	1.1 E-9	59.3
128	7.3 E-7	8.0	1.5 E-10	31.6	1.8 E-11	61.7
256	9.2 E-8	8.0	4.6 E-12	31.8	2.8 E-13	63.0
512	1.2 E-8	8.0	1.4 E-13	32.0	4.4 E-15	62.5

The integrand satisfies the conditions (2) and (10) with $\nu = 1$ for an arbitrary integer $\mu \geq 0$. We compute the integral by the cubature formula (9) corresponding to Gaussian quadrature with 3 knots. Then $m = 3$ and $\mu = 5$. The errors $\varepsilon_N = |Q_N + R_N + S_N|$ and their ratios $\varrho_N = \varepsilon_{N/2}/\varepsilon_N$ for different values of r are presented in Table 1. It follows from the estimates (11) that for $r = 3$, $r = 5$ and $r = 7$ the ratios ϱ_N should be approximately 8, 32, and 64. Computed ϱ_N agrees well with the theoretical convergence rate.

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Kahemõõtmeline kvadratuurvalem ühes punktis iseärasusega funktsioonide jaoks

Enn Tamme

On vaadeldud integraalide arvutamist ruudukujulises piirkonnas funktsioonidest, millel ruudu ühes tipus on nõrk iseärasus, ja uuritud kubatuurvalemit, mille saab, kui kasutada kummaski suunas liitkvadratuurvalemit ebaühtlasel võrgul. On selgitatud kubatuurvalemi vea sõltuvus võrgu ebaühtlusest ja näidatud, millise võrgu korral on saavutatav suurim võimalik koonduvuskiirus. Teoreetilisi tulemusi on kontrollitud numbrilistes näidetes Gaussi liitkvadratuurvalemi korral.