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NUMERICAL COMPUTATION OF WEAKLY SINGULAR INTEGRALS

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Abstract. Numerical evaluation of weakly singular integrals with composite quadrature rules on graded grids is considered. The dependence of the error of the quadrature rule on nonuniformity of the grid is studied. The conditions under which a quadrature rule with nonuniform grid converges in case of a singular integrand with the same rate as the same rule with uniform grid does in case of a smooth integrand are discussed. Theoretical results are verified by numerical examples in case of the composite Gaussian quadrature rule and composite Simpson's rule.

Key words: weakly singular integral, composite quadrature rule.

1. INTRODUCTION

We consider numerical evaluation of integrals

$$\int_0^b f(x)dx \quad (b > 0), \tag{1}$$

where the integrand $f(x)$ can have singularity only at 0. We assume that $f \in C^{k,\nu}(0,b]$ [1], i.e. that $f(x)$ is k times, $k \geq 1$, continuously differentiable for $x \in (0,b] = \{x\colon\ 0 < x \leq b\}$ and that in this domain

$$|f^{(i)}(x)| \leq c \begin{cases} 1 & \text{if} \quad i < 1-\nu, \\ 1 + |\log x| & \text{if} \quad i = 1-\nu, \\ x^{1-\nu-i} & \text{if} \quad i > 1-\nu, \end{cases} \tag{2}$$

where $i = 0, 1, \ldots, k$ and index singularity $\nu < 2$. If $\nu \geq 1$, then $f(x)$ can be unbounded at 0; for $\nu < 1$ it is bounded but its derivatives can be unbounded. For $\nu < 1$ we take $f(x)$ continuous on $[0, b] = \{x\colon\ 0 \leq x \leq b\}$.

We list some typical functions satisfying the assumptions (2).

1) The functions $f(x) = x^\alpha g(x)$ satisfy the conditions (2) with $\nu = 1 - \alpha$ if $\alpha > -1, \alpha \neq 0, g \in C^k(0, b]$ and

$$|g^{(i)}(x)| \leq cx^{-i} \quad \text{for} \quad (0, b], \quad i = 0, 1, \ldots, k.$$

2) The functions of the form $f(x) = x^m \log(x)\, g(x)$ satisfy the conditions (2) with $\nu = 1 - m$ if m is a nonnegative integer and $g \in C^k[0, b]$.

3) The functions $x^\alpha (\log x)^m g(x)$ satisfy the conditions (2) with $\nu = 1 - \alpha + \varepsilon$ if $\alpha > -1$, m is a positive integer, and $g \in C^k[0, b]$. Here ε is an arbitrary (small) positive constant such that $1 - \alpha + \varepsilon < 2$.

The numerical treatment of weakly singular integrals is studied, for example, in [2]. The use of the product integration method for the evaluation of such integrals is discussed in [3–5]. The computation of weakly singular integrals with trapezoidal rule and with Gaussian quadratures on graded grids is considered respectively in [2,6] and [7]. The present paper deals with the computation of weakly singular integrals with composite quadrature formulas on graded grids. As opposed to other available results about high-order numerical methods, this one is fully discrete; it does not assume that certain integrals can be computed exactly. It is shown under which conditions a quadrature rule with nonuniform grid converges in case of a singular integrand with the same rate as the same rule with uniform grid does in case of a smooth integrand. The computation of integrals with composite quadrature rules is simpler than with product integration methods, but for the evaluation of the integral with the same accuracy it is necessary to use a more nonuniform grid.

At the end of the paper theoretical results are verified by numerical examples in case of the composite Gaussian quadrature rule and composite Simpson's rule.

2. THE CONVERGENCE RATE OF COMPOSITE QUADRATURE RULES

We use a quadrature formula

$$\int_{-1}^{1} \Psi(x)dx \approx \sum_{q=1}^{m} w_q \Psi(\xi_q) \tag{3}$$

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

$$-1 \leq \xi_1 < \xi_2 < \ldots < \xi_m \leq 1.$$

We divide the interval $[0,b]$ of integration with grid points

$$x_j = b\left(\frac{j}{N}\right)^r, \quad j = 0,1,\dots,N,$$

into N subintervals $[x_{j-1},x_j]$, $j=1,\dots,N$. Here the real number $r \geq 1$ characterizes the nonuniformity of the grid. If $r=1$, then the grid points are uniformly located. Note that $x_0 = 0$ and $x_N = b$. For the evaluation of the integral (1) we use the composite quadrature rule

$$\int_0^b f(x)dx = x_1 f(\xi) + \sum_{j=2}^{N} \frac{x_j - x_{j-1}}{2} \sum_{q=1}^{m} w_q f(\xi_{jq}) + \mathcal{R}_N, \tag{4}$$

where $\xi = x_1/2$ and

$$\xi_{jq} = x_{j-1} + \frac{\xi_q + 1}{2}(x_j - x_{j-1}). \tag{5}$$

Note that on the first interval $[0,x_1]$ the rectangular rule and on the intervals $[x_{j-1},x_j]$, $j=2,\dots,N$, the quadrature rule (3) is used.

About the convergence rate of the quadrature rule (4) the following result holds.

Theorem 1. *Assume that the quadrature formula* (3) *is exact for all polynomials of degree* μ, $f \in C^{\mu+1,\nu}$, $0<\nu<2$ *and* $m-1 \leq \mu \leq 2m-1$. *Then for the error* $\mathcal{R}_N$ *of the quadrature rule* (4) *the following estimates hold*

$$|\mathcal{R}_N| \leq c \begin{cases} N^{-r(2-\nu)+1} & \text{if} \quad 1 \leq r \leq \dfrac{\mu+2}{2-\nu}, \\ N^{-\mu-1} & \text{if} \quad r \geq \dfrac{\mu+2}{2-\nu}. \end{cases} \tag{6}$$

Proof. We use some ideas from [1]. In addition to the knots $\xi_1,\dots,\xi_m$, we fix in the interval $(-1,1)$ $\mu-m+1$ knots $\xi_{m+1},\dots,\xi_{\mu+1}$ so that $\xi_i \neq \xi_j$ if $i \neq j$ and generate by the formula (5) the corresponding knots $\xi_{jq} \in (x_{j-1},x_j)$, $q=m+1,\dots,\mu+1$, $j=2,\dots,N$. We define the interpolation projector $\mathcal{P}_N$ by the formula

$$(\mathcal{P}_N f)(x) = \sum_{q=1}^{\mu+1} f(\xi_{jq})\varphi_{jq}(x), \quad x \in [x_{j-1},x_j],\ j=2,\dots,N,$$

where $\varphi_{jq}(x)$ are the polynomials of degree μ such that

$$\varphi_{jq}(\xi_{jp}) = \begin{cases} 1 & \text{if} \quad p=q, \\ 0 & \text{if} \quad p \neq q,\ p=1,\dots,\mu+1. \end{cases}$$

Then $(\mathcal{P}_N f)(\xi_{jq}) = f(\xi_{jq})$, $q = 1, \dots, \mu+1$, $j = 2, \dots, N$, and $(\mathcal{P}_N f)(x)$ is on $[x_{j-1}, x_j]$, $j = 2, \dots, N$, the polynomial of the degree not exceeding μ. Due to the exactness of the formula (3), for the polynomials of degree μ we have

$$\int_{x_{j-1}}^{x_j} (\mathcal{P}_N f)(x)dx = \frac{x_j - x_{j-1}}{2} \sum_{q=1}^{m} w_q f(\xi_{jq}), \quad j = 2, \dots, N.$$

Therefore the error $\mathcal{R}_N$ of the quadrature rule (4) is given by

$$\mathcal{R}_N = \int_0^{x_1} [f(x) - f(\xi)]dx + \sum_{j=2}^{N} \int_{x_{j-1}}^{x_j} [f(x) - (\mathcal{P}_N f)(x)]dx, \tag{7}$$

where $\xi = x_1/2$.

First of all we estimate the first integral in (7). As

$$f(x) - f(\xi) = \int_\xi^x f'(s)ds, \quad x \in (0, x_1],$$

then

$$\int_0^{x_1} [f(x) - f(\xi)]dx = \int_0^\xi \int_\xi^x f'(s)dsdx + \int_\xi^{x_1} \int_\xi^x f'(s)dsdx$$

$$= -\int_0^\xi sf'(s)ds + \int_\xi^{x_1} (x_1 - s)f'(s)ds.$$

Thus

$$\left| \int_0^{x_1} [f(x) - f(\xi)]dx \right| \le \int_0^\xi s|f'(s)|ds + \int_\xi^{x_1} (x_1 - s)|f'(s)|ds$$

$$\le \int_0^{x_1} s|f'(s)|ds \le c \int_0^{x_1} s^{1-\nu}ds = \frac{c}{2-\nu} x_1^{2-\nu},$$

i.e.

$$\left| \int_0^{x_1} [f(x) - f(\xi)]dx \right| \le c_1 x_1^{2-\nu}. \tag{8}$$

Now we estimate the remaining integrals in (7). Let $v(x)$ be an arbitrary polynomial of degree μ on $[x_{j-1}, x_j]$, $j = 2, \ldots, N$. Then, for $x \in [x_{j-1}, x_j]$, $(\mathcal{P}_N v)(x) = v(x)$ and

$$|f(x) - (\mathcal{P}_N f)(x)| \le |f(x) - v(x)| + |(\mathcal{P}_N v)(x) - (\mathcal{P}_N f)(x)|.$$

As in [8] we obtain

$$\sup_{x_{j-1}<x<x_j} |(\mathcal{P}_N v)(x) - (\mathcal{P}_N f)(x)| \le c \sup_{x_{j-1}<x<x_j} |v(x) - f(x)|,$$

where the constant c does not depend on j and N, then

$$\sup_{x_{j-1}<x<x_j} |f(x) - (\mathcal{P}_N f)(x)| \le (1+c) \sup_{x_{j-1}<x<x_j} |f(x) - v(x)|, \; j = 2, \ldots, N. \tag{9}$$

If $v(x)$ is the Taylor polynomial

$$v(x) = \sum_{i=0}^{\mu} \frac{1}{i!} f^{(i)}(x_j)(x - x_j)^i,$$

then, due to (2),

$$|f(x) - v(x)| = \frac{1}{\mu!}\Big|\int_x^{x_j} (x-s)^\mu f^{(\mu+1)}(s)ds\Big| \le \frac{c}{\mu!}\int_x^{x_j} (s-x)^\mu s^{-\mu-\nu} ds,$$

$$x \in [x_{j-1}, x_j].$$

Since here $0 \le s - x \le x_j - x_{j-1}$ and $x_j \ge s \ge x_{j-1} \ge 2^{-r} x_j$, it follows that

$$\sup_{x_{j-1}<x<x_j} |f(x) - v(x)| \le c_2 (x_j - x_{j-1})^{\mu+1} x_j^{-\mu-\nu}$$

and with the help of (9) we get

$$\int_{x_{j-1}}^{x_j} |f(x) - (\mathcal{P}_N f)(x)| dx \le c_3 (x_j - x_{j-1})^{\mu+2} x_j^{-\mu-\nu}, \quad j = 2, \ldots, N. \tag{10}$$

From formulas (7), (8), and (10) it now follows that

$$|\mathcal{R}_N| \le c_4 \Big[x_1^{2-\nu} + \sum_{j=2}^{N} (x_j - x_{j-1})^{\mu+2} x_j^{-\mu-\nu} \Big].$$

As $x_j = b(j/N)^r$ and $0 < x_j - x_{j-1} \le b\, r\, j^{r-1}/N^r$, we have

$$|\mathcal{R}_N| \le c_5 \Big[N^{-r(2-\nu)} + N^{-r(2-\nu)} \sum_{j=2}^{N} j^{r(2-\nu)-\mu-2} \Big].$$

If $r(2-\nu) \leq \mu+2$, then

$$\sum_{j=2}^{N} j^{r(2-\nu)-\mu-2} \leq N$$

and

$$|\mathcal{R}_N| \leq cN^{-r(2-\nu)+1}.$$

But if $r(2-\nu) \geq \mu+2$, then

$$\sum_{j=2}^{N} j^{r(2-\nu)-\mu-2} \leq N^{r(2-\nu)-\mu-1}$$

and we get

$$|\mathcal{R}_N| \leq cN^{-\mu-1}.$$

Theorem 1 is proved.

Remark. If $1 < \nu < 2$, then

$$\Big|\int_0^{x_1} f(x)dx\Big| \leq c\int_0^{x_1} x^{1-\nu}dx = \frac{c}{2-\nu}x_1^{2-\nu}$$

and the estimates (6) hold also in the case when on the first interval $[0, x_1]$ the integrand $f(x)$ is replaced with 0, i.e. for the error $\mathcal{R}_N$ of the quadrature rule

$$\int_0^b f(x)dx = \sum_{j=2}^{N} \frac{x_j - x_{j-1}}{2} \sum_{q=1}^{m} w_q f(\xi_{jq}) + \mathcal{R}_N. \tag{11}$$

Although the convergence rate of this quadrature rule is almost the same as that of the quadrature rule (4), the rule (4) usually approximates the integral (1) a little better. Note that in [7] the convergence of the quadrature rule (11) corresponding to the Gaussian quadrature (3) is studied and for this particular case the second from the estimates (6) is proved.

If $\nu < 1$, then the integrand $f(x)$ is continuous on $[0, b]$ and it is appropriate to use formula (3) also on $[0, x_1]$, i.e. we can use for the integral (1) the composite quadrature rule

$$\int_0^b f(x)dx = \sum_{j=1}^{N} \frac{x_j - x_{j-1}}{2} \sum_{q=1}^{m} w_q f(\xi_{jq}) + \mathcal{R}_N, \tag{12}$$

where the knots ξ_{jq} are calculated by (5). For this rule the following result holds.

Theorem 2. *Assume that quadrature formula* (3) *is exact for all polynomials of degree* μ, $f \in C^{\mu+1,\nu}$, $\nu < 1$ *and* $m-1 \le \mu \le 2m-1$. *Then the error* $\mathcal{R}_N$ *of the quadrature rule* (12) *satisfies in the case* $\nu > -\mu$ *the estimates* (6), *in the case* $\nu = -\mu$ *the estimates*

$$|\mathcal{R}_N| \le c \begin{cases} N^{-\mu-1} \log N & \text{if} \quad r = 1, \\ N^{-\mu-1} & \text{if} \quad r > 1, \end{cases}$$

and in the case $\nu < -\mu$ *the estimate*

$$|\mathcal{R}_N| \le c N^{-\mu-1} \quad \text{if} \quad r \ge 1.$$

Proof. As in the proof of Theorem 1 we can show that the error $\mathcal{R}_N$ of the quadrature rule (12) is given by

$$\mathcal{R}_N = \sum_{j=1}^{N} \int_{x_{j-1}}^{x_j} [f(x) - (\mathcal{P}_N f)(x)] dx$$

and that

$$\sup_{x_{j-1}<x<x_j} |f(x) - (\mathcal{P}_N f)(x)| \le c \sup_{x_{j-1}<x<x_j} \int_x^{x_j} (s-x)^{\mu} |f^{(\mu+1)}(s)| dx, \tag{13}$$
$$j = 1, \ldots, N.$$

It follows immediately from (13) and (2) that for $j = 2, \ldots, N$

$$\int_{x_{j-1}}^{x_j} |f(x) - (\mathcal{P}_N f)(x)| dx \le c_1 (x_j - x_{j-1})^{\mu+1} \begin{cases} 1 & \text{if} \quad \mu < -\nu, \\ 1 + |\log x_j| & \text{if} \quad \mu = -\nu, \\ x_j^{-\mu-\nu} & \text{if} \quad \mu > -\nu. \end{cases} \tag{14}$$

We will show that (14) holds also for $j = 1$. Substituting $x = \eta x_1$ and $s = \sigma x_1$, we get

$$\sup_{0<x<x_1} \int_x^{x_1} (s-x)^{\mu} \big| f^{(\mu+1)}(s) \big| dx$$
$$\le c_2 \sup_{0<x<x_1} \int_x^{x_1} (s-x)^{\mu} \left\{ \begin{array}{lll} 1 & \text{if} & \mu < -\nu \\ 1 + |\log s| & \text{if} & \mu = -\nu \\ s^{-\mu-\nu} & \text{if} & \mu > -\nu \end{array} \right\} ds$$
$$= c_2 x_1^{\mu+1} \sup_{0<\eta<1} \int_\eta^1 (\sigma - \eta)^{\mu} \left\{ \begin{array}{lll} 1 & \text{if} & \mu < -\nu \\ 1 + |\log(\sigma x_1)| & \text{if} & \mu = -\nu \\ (\sigma x_1)^{-\mu-\nu} & \text{if} & \mu > -\nu \end{array} \right\} d\sigma$$

and the estimates (14) for $j=1$ are deduced from

$$\sup_{0<\eta<1} \int_\eta^1 (\sigma-\eta)^\mu \sigma^{-\mu-\nu} d\sigma \le \int_0^1 \sigma^{-\nu} d\sigma = \frac{1}{1-\nu}$$

when $\mu \ge 0$ and $\nu < 1$.

Now the estimates of Theorem 2 follow analogously to the ones of Theorem 1.

3. NUMERICAL EXAMPLES

Consider the computation of the integrals

$$\int_0^1 \frac{(\ln x)^3}{1+x} dx = -\frac{7}{120}\pi^4 \tag{15}$$

and

$$\int_0^1 \frac{dx}{\sqrt{x}} = 2. \tag{16}$$

The integrands of the integrals (15) and (16) belong respectively to $C^{k,1+\varepsilon}(0,1]$ and to $C^{k,1.5}(0,1]$ for an arbitrary positive integer k and for an arbitrary $\varepsilon \in (0,1)$. These integrals with the composite quadrature rule (4) corresponding to Gaussian quadrature with 3 knots and to Simpson's rule are calculated using respectively $3N-2$ and $2N$ values of the integrands. In Table 1 and Table 2 the errors $|\mathcal{R}_N|$ of the integrals (15) and (16) and their ratios $\varrho_N = |\mathcal{R}_{N/2}/\mathcal{R}_N|$ are presented. For Simpson's rule $\mu = 3$ and from the estimates (6) it follows that for $r=6$ in Table 1 and for $r=10$ in Table 2 the ratios ϱ_N should be approximately 16, which agrees very well with the actual convergence rate. For Gaussian quadrature with 3 knots $\mu = 5$ and from the estimates (6) it follows that for $r=8$ in Table 1 and for $r=14$ in Table 2 the ratio ϱ_N should be approximately 64. When $r < (\mu+2)/(2-\nu)$, then approximate values of the integrals converged somewhat quicker than the estimates (6) guaranteed.

When we used for computing the integral (15) the quadrature rules (11) and (12) for $r=5$ instead of the quadrature rule (4) corresponding to Gaussian quadrature, then in the first case we got approximate values of the integral with somewhat greater errors and in the second case with somewhat smaller errors than those displayed in Table 1. In the other cases presented in Tables 1 and 2 the rules (11) and also (12) corresponding to Gaussian quadrature gave the approximate values of the integrals nearly with the same errors as those shown in the tables.

Table 1. The errors $|\mathcal{R}_N|$ and their ratios ϱ_N for the integral (15)

N	Gaussian quadrature with 3 knots				Simpson's rule	
	$r=5$		$r=8$		$r=6$	
	$\lvert\mathcal{R}_N\rvert$	ϱ_N	$\lvert\mathcal{R}_N\rvert$	ϱ_N	$\lvert\mathcal{R}_N\rvert$	ϱ_N
8	1.4 E−2		1.3 E−2		1.2 E−1	
16	8.6 E−4	16.5	3.7 E−4	36.1	9.5 E−3	12.8
32	4.5 E−5	19.1	7.6 E−6	48.6	6.6 E−4	14.4
64	2.2 E−6	21.0	1.3 E−7	56.3	4.3 E−5	15.3
128	1.0 E−7	22.5	2.2 E−9	60.5	2.8 E−6	15.7
256	4.1 E−9	23.6	3.6 E−11	62.5	1.7 E−7	15.9
512	1.7 E−10	24.5	5.6 E−13	63.5	1.1 E−8	16.0

Table 2. The errors $|\mathcal{R}_N|$ and their ratios ϱ_N for the integral (16)

N	Gaussian quadrature with 3 knots				Simpson's rule	
	$r=10$		$r=14$		$r=10$	
	$\lvert\mathcal{R}_N\rvert$	ϱ_N	$\lvert\mathcal{R}_N\rvert$	ϱ_N	$\lvert\mathcal{R}_N\rvert$	ϱ_N
8	3.3 E−3		8.0 E−3		3.8 E−2	
16	1.4 E−4	22.7	2.7 E−4	30.1	2.8 E−3	13.3
32	5.2 E−6	27.6	5.8 E−6	45.7	2.0 E−4	14.5
64	1.8 E−7	29.9	1.1 E−7	54.7	1.3 E−5	15.2
128	5.6 E−9	31.0	1.9 E−9	59.3	8.3 E−7	15.6
256	1.8 E−10	31.5	2.9 E−11	61.7	5.2 E−8	15.8
512	5.6 E−12	31.7	4.6 E−13	62.8	3.3 E−9	15.9

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NÕRGALT SINGULAARSETE INTEGRAALIDE LIGIKAUDNE ARVUTAMINE

Enn TAMME

On vaadeldud nõrgalt singulaarsete integraalide arvutamist ebaühtlast võrku kasutavate liitkvadratuurvalemite abil. On selgitatud kvadratuurvalemi vea sõltuvus võrgu ebaühtlusest ja näidatud, millise ebaühtlase võrgu puhul kvadratuurvalem koondub nõrgalt singulaarse integreeritava funktsiooni korral sama kiiresti kui sileda funktsiooni korral ühtlasel võrgul. Teoreetilisi tulemusi on kontrollitud numbrilistes näidetes, kasutades Gaussi ja Simpsoni kvadratuurvalemeid.