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ON INTEGRATION OF NEARLY SINGULAR FUNCTIONS BY THE QUADRATURES OVER THE SEMICIRCLE WITH EQUAL WEIGHTS

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Abstract. *The serious defects of the classical quadratures can be seen in integration of the functions which have singularities near the interval of integration, named nearly singular functions. In this paper, we show that, for numerical integral evaluating, very effectively the quadratures over the semicircle with the equal weights can be used. We illustrate the previous considerations by the numerical examples.*

1. INTRODUCTION

One of the main problems in mathematical software is the choice of a method for numerical evaluating of integrals by computer. The serious defects of the classical quadratures can be seen in integration of the functions which have singularities near the interval of inte-gration, named *nearly singular functions*.

We suppose that $K(x)$ is a function of the next two possible forms:

$$K_1(x) = \frac{1}{x \pm (1+\delta)}, \; K_2(x) = \frac{1}{x^2 + \delta^2}, \tag{1.1}$$

where δ is a small positive number. We consider integrals of the type

$$\int_{-1}^{1} f(x) K(x) dx, \tag{1.2}$$

where $f(x)$ is a smooth function on (-1, 1).

Newton-Cotes' and Gauss' quadratures are widely used in numerical integration. They are included in most computer programs. But, using these formulas, we get very bad approximations for integrals of the type (1.2).

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Example 1.1. Like an illustration, we consider the integral

$$\int_{-1}^{1} \frac{1}{x^2+2^{-2m}}\, dx = 2^{m+1} \arctan 2^m .$$

Using the classical Gauss-Legendre's quadrature, we obtain the next table of relative errors:

m	exact value	rell. err. for $n = 10$	rell. err. for $n = 20$
1	4.42859487	0.114705(−3)	0.762228(−8)
2	10.606541	0.129672(−1)	0.926745(−4)
3	23.143061	0.147235	0.129893(−1)
4	48.268081	0.441472	0.149233
5	98.531616	0.696737	0.443436
7	400.12390	0.922650	0.845359
9	1606.4954	0.980691	0.961166

We see that, as the singular point tends to the interval (-1,1), the accuracy is worse, so in the last column there are no correct digits in the approximation.

T. Hasegawa and T. Torii, in their paper [2], expanded the function $f(x)$ in terms of the Chebyshev polynomials.

Example 1.2. T. Hasegawa and T. Torii noticed that the function $f(x) = (1-a^2)/(1-2ax+a^2)$ has a Chebyshev series expansion

$$f(x) = T_0(x) + 2\sum_{n=1}^{\infty} a^n T_n(x) \quad (|a| < 1),$$

but, when a is close to **1**, this series converges slowly and the numerical integration of the integrals (1.2) by their method is difficult.

Gautschi and Milovanović, in their papers [1] , [3] and [4], introduced and applied the quadratures of Gaussian type over the unit semicircle.

In this paper, we show that, for numerical integral evaluating, very effectively the quadratures over the semicircle with the equal weights can be used.

The quadratures of this type have lower algebraic degree of accuracy, but there are cases when they are more successful.

Preferences of the quadrature with equal weights can be seeen in the next situations:

(1) when the rounding error of evaluating $f(z)$ in the nodes is significantly greater than the error of method $E_n(f)$;

(2) when the error of the product of the coefficients and values $f(z)$ in the nodes is large, so the reduction of the number of operations is very useful.

2. The quadrature over the semicircle with equal weights

Let us construct a quadrature of the form

$$\int_{\Gamma} f(z) w(z) \frac{dz}{iz} = A_n \sum_{k=1}^{n} f(z_k) + E_n(f), \tag{2.1}$$

where

$$.\Gamma = \{z \in C: \quad z = e^{i\theta}, \quad 0 \le \theta \le \pi\}$$

is a upper unit semicircle, which has the greatest algebraic degree of accuracy,

$$.E_n(z^m) = 0, \quad m = 0,1,\ldots,n. \tag{2.2}$$

Let μ_m be a moment of order m defined by:

$$\mu_m = \int_\Gamma z^m w(z) \frac{dz}{iz}.$$

From (2.2), we obtain a system of nonlinear algebraic equations

$$A_n \sum_{k=1}^{n} z_k^m = \mu_m, \quad m = 0,1,\ldots,n.$$

For $m = 0$, we have $\boldsymbol{n A_n = \mu_0}$, i.e. $\boldsymbol{A_n = \mu_0 / n}$.
Denoting by

$$s_m = \sum_{k=1}^{n} z_k^m, \quad m = 1,\ldots,n.$$

we get $A_n\, s_m = \mu_m$, i.e. $s_m = n\, \mu_m / \mu_0$. Then, the coefficients of the polynomial

$$P_n(z;w) = \prod_{k=1}^{n} (z - z_k) = z^n + a_1 z^{n-1} + \cdots + a_{n-1} z + a_n$$

can be found from the Newton's identities

$$s_m + s_{m-1} a_1 + \cdots + s_1 a_{m-1} + m a_m = 0, \quad m = 0,1,\ldots,n.$$

Numerical evaluation of the nodes z_k like the zeros of $P_n(z;w)$, can be done, for example, by Weierstrass' simultaneous method

$$z_i^{(k+1)} = z_i^{(k)} - \frac{P_n(z_i^{(k)}; w)}{\prod_{m=1, m\ne i}^{n} (z_i^{(k)} - z_m^{(k)})} \quad (i = 1,\ldots,n; \quad k = 0,1,\ldots),$$

starting with

$$z_k^{(0)} = e^{i\pi k/n}, \quad k = 1,\ldots,n.$$

So, the quadrature (2.1) is completed.

3. The quadrature in Legendre's case

Let us consider the case $w(z) = 1$. Then, the moments are

$$\mu_m = \int_\Gamma z^m \frac{dz}{iz} = \begin{cases} \pi, & m = 0 \\ 0, & m - even \\ 2i/\pi, & m - odd. \end{cases}$$

The weight of quadrature has the value $A_n = \pi / n$ and the values s_m are

$$s_m = \begin{cases} 0, & m - even \\ 2ni/(m\pi), & m - odd. \end{cases}$$

The sequence of coefficients a_k (k = 1,2, …,n), can be generated by

$$a_1 = -i\frac{2n}{\pi},$$

$$a_{2m} = \frac{n}{m\pi}\sum_{k=1}^{m}\frac{\operatorname{Im}(a_{2m-2k+1})}{2k-1},$$

$$a_{2m+1} = -i\frac{2n}{(2m+1)\pi}\left\{\frac{1}{2m+1}+\sum_{k=1}^{m}\frac{a_{2m-2k+2}}{2k-1}\right\}, \quad m = 1,2,\ldots.$$

Table 3.1. The coeficients and nodes of the quadrature over the unit semicircle with equal weights.

n	k	z_k	A_n
2	1,2	⌒0.636619772410672 + 0.636619772410672 i	1.5707963267948970
3	1	1.033527353077526 i	1.047197580337524
	2,3	⌒0.852102589246862 + 0.438165981981385 i	
4	1,2	⌒0.907093571729045 + 0.312582167894042 i	0.7853981852531433
	3,4	⌒0.444692518110112 + 0.960657364550442 i	
5	1,2	⌒0.924842395931091 + 0.251320138657836 i	0.6283185482025146
	3	1.069071315376234 i	
	4,5	⌒0.654787741912245 + 0.805981759444682 i	
10	1,2	⌒0.974689431224249 + 0.125340283287261 i	0.3141592741012573
	3,4	⌒0.934303434051705 + 0.447067653489433 i	
	5,6	⌒0.730556937949320 + 0.762038455038208 i	
	7,8	⌒0.397934437066345 + 0.953808496484562 i	
	9,10	⌒0.000000839311565 + 0.985558937810959 i	
20	1,2	⌒1.015089408516857 + 0.223486600123878 i	0.1570796370506287
	3,4	⌒1.002358060993204 + 0.433537160342106 i	
	5,6	⌒0.991031661357507 + 0.059020872735738 i	
	7,8	⌒0.935940329188950 + 0.657072934760004 i	
	9,10	⌒0.808731587799988 + 0.868276524069418 i	
	11,12	⌒0.710132748890758 + 0.276482223452862 i	
	13,14	⌒0.624372917927863 + 1.046965421012197 i	
	15,16	⌒0.394277280445374 + 1.176360522475909 i	
	17,18	⌒0.248049591431190 + 0.380730790885576 i	
	19,20	⌒0.134797594666668 + 1.244263033729825 i	

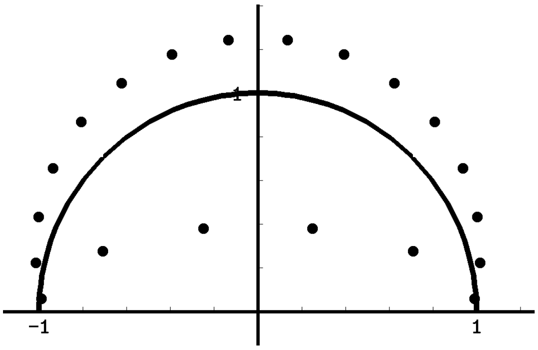

Fig. 3.1. The nodes of the quadrature over the unit semicircle with equal weights.

4. EXAMPLES

In order to apply the quadrature with equal weights on the semicircle to Example 1.1., we start by Cauchy's residual theorem for the function $F(z) = 1/(z^2 + 2^{-2m})$,

$$\int_{[-1,1]} F(x)dx + \int_{\Gamma} F(z)dz = 2\pi i \ \mathrm{Res}\ F(2^{-m} i) = 2^m \pi.$$

Hence

$$\int_{-1}^{1} \frac{1}{x^2 + 2^{-2m}} dx \approx 2^m \pi - i\frac{\pi}{n}\sum_{k=1}^{n} f(z_k),$$

with $f(z) = z/(z^2 + 2^{-2m})$.

The quadrature with equal weights on the semicircle gives much better accuracy, as it is shown in the next table.

Table 4.1. The quadrature with equal weights on the semicircle applied, on Example 1.1. .

m	exact value	rel. error for n = 10	rel. error for n = 20
4	48.268081	0.956077(−3)	0.309188(−3)
5	98.531616	0.448527(−3)	0.118221(−3)
6	199.06209	0.219572(−3)	0.546025(−4)
7	400.12390	0.108935(−3)	0.266841(−4)
8	802.24773	0.542938(−4)	0.132490(−4)
9	1606.4954	0.271084(−4)	0.660881(−5)

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INTEGRACIJA SKORO-SINGULARNIH FUNKCIJA POMOĆU KVADRATURA NA POLUKRUGU SA JEDNAKIM TEŽINAMA

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Ozbiljni nedostaci klasičnih kvadraturnih formula mogu se zapaziti kod integracije funkcija koje imaju singularitete u blizini intervala integracije, tzv. skoro-singularnih funkcija. Neke metode za izračunavanje takvih integrala su razvili T. Hasegava i T. Torii. U radu pokazujemo da se za izračunavanje takvih integrala, vrlo efikasno mogu upotrebiti kvadrature na polukrugu Gaussovog tipa ili kvadrature sa jednakim koeficijentima. Ove druge imaju niži algebarski stepen tačnosti, ali postoje brojni slučajevi kada su one uspešnije, posebno za funkcije sa većom greškom zaokruživanja u čvorovima nego što je greška metode. Prethodna razmatranja ilustrujemo numeričkim primerima.