Int. J. Contemp. Math. Sciences, Vol. 3, 2008, no. 23, 1133 - 1140

High-Order Corrected Trapezoidal Quadrature Rules for Functions with a Logarithmic Singularity on a Circle[1]

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Abstract

In this report we construct high-order quadrature rules to evaluate integrals of the form

$$J(v) = \int_{-\pi}^{\pi} v(\theta)\log(\omega(1-\cos(\theta))d\theta,$$

where v is a C^∞ periodic function of period 2π, and ω is a positive constant. The constructions of the quadratures are based on the method of central corrections described in [4]. The quadratures consist of the trapezoidal rule plus a local weighted sum of the values of v around the point of singularity. Integrals of the above type appear in scattering calculations; we test the performance of the quadrature rules with an example of this kind.

Mathematics Subject Classification: 65D30

Keywords: Quadrature rule, Corrected trapezoidal rule, Logarithmic singularity, Central corrections

1 Introduction

Corrected trapezoidal quadrature rules have been applied to approximate the numerical solution of integral equations related to scattering calculations (see [1], [2]). We consider in this paper corrected trapezoidal quadrature rules to approximate integrals of the form

$$J(v) = \int_{-\pi}^{\pi} v(\theta)\log(\omega(1-\cos(\theta))d\theta, \tag{1}$$

[1]This work was supported by Asociación Mexicana de Cultura A.C.

where v is a smooth function of period 2π and ω is a positive real number. Integrals of the type (1) can be applied to the direct acoustic obstacle scattering problem in $\mathbb{R}^2$ (see [3]). Such problem involves calculations of integrals of the form

$$g(t) = \int_0^{2\pi} v(\theta)\log(4\sin^2(\frac{t-\theta}{2}))d\theta = \int_{-\pi}^{\pi} v(\theta)\log(2(1-\cos(t-\theta)))d\theta, \quad (2)$$

where v is a periodic smooth function of period 2π, and $t \in [0, 2\pi]$. The quadratures we consider are also useful to calculate path integrals of the type $\int_{C_R} f(x,y)\log(|(x_0,y_0)-(x,y)|)ds$ where C_R is a circle of radius R and $(x_0,y_0) \in C_R$. These integrals take the form $\int_{-\pi}^{\pi} v(\theta)\log(\omega(1-\cos(\theta_0-\theta)))d\theta$, where v has period 2π and $\omega = 2R^2$. A stable, accurate, and efficient evaluation of integrals of the type (1) is desirable in such applications. In [4] it is described a corrected trapezoidal quadrature rule to approximate integrals with a logarithmic singularity in 1-D. The method we use is an adaptation of the method of central corrections of [4] for logarithmic singularities. The quadrature rules obtained this way remain stable for high-orders and involve the trapezoidal rule plus a weighted sum of a few values of v around 0.

The paper is organized as follows: Section 2 contains notation and some properties of the trapezoidal rule. Section 3 describes how to build the quadratures to approximate (1). Section 4 tests the quadratures and describes how to apply them to approximate a convolution of the type (2).

2 The trapezoidal rule

For the remaining of this report $I = [-\pi, \pi]$, $v : \mathbb{R} \to \mathbb{R}$ will be a C^∞ function, and $f : \mathbb{R}\backslash\{0\} \to \mathbb{R}$ a function defined as

$$f(x) = v(x)\log(\omega(1-\cos(x))). \quad (3)$$

Therefore our goal is to approximate the integral

$$\int_I f(x)dx = \int_I v(x)\log(\omega(1-\cos(x)))dx \quad (4)$$

using a corrected trapezoidal rule. For this purpose we first discretize the interval I using a uniform grid containing $n+1$ points. Thus $h = 2\pi/n$ is the distance between sampling points. We will assume that n is even so that 0 is one of the sampling points.

The trapezoidal rule applied to a function $u : \mathbb{R} \to \mathbb{R}$ on the interval I and with respect to the uniform partition $\{x_j\}$, $x_j = -\pi + jh$, will be denoted by

$T_h(u)$, and it is defined as

$$T_h(u) = h\left(\sum_{j=1}^{n-1} u(x_j) + \frac{1}{2}(u(x_0) + u(x_n))\right), \tag{5}$$

As it is well-known, if the function u has $2m$ continuous derivatives and if u is periodic in $\mathbb{R}$ with period equal to the length of the interval I then it follows from the Euler-Maclaurin formula that $T_h(u)$ converges to the integral $\int_I u(x)dx$ at the rate

$$\int_I u(x)dx - T_h(u) = O(h^{2m}). \tag{6}$$

If u is either non-smooth or non-periodic then $\int_I u(x)dx - T_h(u)$ is at most $O(h^2)$. Since the type of functions f we want to integrate in this report are non-smooth due to the logarithmic singularity at 0, the trapezoidal rule yields a poor approximation to the integrals.

In the method of central corrections (see [4]) there are two type of corrections to the trapezoidal rule:

1) *Boundary correction*
2) *Logarithmic correction*

We will specify in the next section the main aspects of both type of corrections.

3 Boundary and logarithmic correction

The corrected trapezoidal rule with a logarithmic singularity requires two type of corrections. The first correction is on the boundary of the interval I; this correction is used when the integrand f of (4) is non-periodic. The second type of correction is due to the point singularity of logarithm at 0.

3.1 Boundary correction

Boundary correction is defined as follows: let m be a positive odd integer and β_k^m, $k = 1, \ldots, (m-1)/2$ be the $(m-1)/2$ coefficients for boundary correction (see [4]). If $\{x_j\}$, $x_j = -\pi + jh = -\pi + 2\pi j/n$, is the grid used to discretize the interval I, with n a positive even integer, and $u : \mathbb{R} \to \mathbb{R}$ a function, then the boundary corrected trapezoidal rule applied to u is denoted by $T^n_{\beta^m}(u)$, and is given by the formula

$$\begin{aligned} T^n_{\beta^m}(u) &= h\left(\sum_{j=1}^{n-1} u(x_j) + \frac{1}{2}(u(x_0) + u(x_n))\right) \\ &+ h\sum_{k=1}^{\frac{m-1}{2}} \left(-u(x_{-k}) + u(x_k) + u(x_{n-k}) - u(x_{n+k})\right)\beta^m_k \end{aligned} \tag{7}$$

Note that if u is periodic with period 2π it follows that $T^n_{\beta^m}(u)$ becomes the trapezoidal rule $T_h(u)$, and in this case the trapezoidal rule can be written as $T_h(u) = h\sum_{j=0}^{n-1} u(x_j)$.

When the function u has $m+1$ continuous derivatives then (see [4])

$$\int_I u(x)dx - T^n_{\beta^m}(u) = O(h^{m+1}). \tag{8}$$

In our case we are interested in applying the boundary corrected trapezoidal rule to a function f of the type (3) which is not defined at 0. For this type of function f we define the punched boundary corrected trapezoidal rule as:

$$T^n_{0,\beta^m}(f) = T^n_{\beta^m}(\tilde{f}) \tag{9}$$

where

$$\tilde{f}(x) = \begin{cases} f(x) & \text{if } x \neq 0 \\ 0 & \text{if } x = 0. \end{cases} \tag{10}$$

Since $\tilde{f}$ is not smooth at 0, the boundary corrected trapezoidal rule $T^n_{\beta^m}(\tilde{f})$ gives a low order approximation to the integral (4). A logarithmic correction term needs to be added to the boundary correction term in order to improve the order of convergence. This correction is described in the next section.

3.2 Logarithmic correction

Logarithmic correction is needed due to the point of singularity of the function f at 0. This type of correction added to the boundary correction $T^n_{0,\beta^m}(f)$ will increase the rate of convergence to the integral (4). If v is the C^∞ function related to f by the formula (3), the logarithmic correction is computed by means of a weighted sum of the values of v at neighboring points of 0. More explicitly, we will find k correction coefficients $c_0, c_1, \ldots, c_{k-1}$ independent of the distance h between sampling points, independent of v (but dependent of k) , so that the logarithmic correction $L^n_{\mathbf{c}^k}(v)$, defined as

$$L^n_{\mathbf{c}^k}(v) = h(\log(\omega h^2) + c_0)v(0) + h\left(\sum_{r=1}^{k-1} c_r(v(-rh) + v(rh))\right), \tag{11}$$

has the property that

$$J(v) = \int_{-\pi}^{\pi} v(\theta)\log(\omega(1-\cos(\theta))d\theta = T^n_{0,\beta^m}(f) + L^n_{\mathbf{c}^k}(v) + O(h^{2k+1}), \quad (12)$$

provided $m > 2k$.

Our interest in this paper is when the function v is smooth and periodic with period 2π; in this case, since boundary correction is not needed, the quadratures take the form

$$J(v) = T_h(\tilde{f}) + L^n_{\mathbf{c}^k}(v) + O(h^{2k+1}). \quad (13)$$

Observe that quadratures (13) are computed with the trapezoidal rule plus a local correction involving only the function v around the point of singularity 0. In the next section we describe how to compute the correction coefficients of the quadratures (13).

3.3 Computation of the logarithmic correction coefficients

In this section we adapt the method of central correction described in [4] to obtain logarithmic correction coefficients required in (13). To compute the first k coefficients $\mathbf{c}^k$ we take as v in Equation (12) the C^∞ monomial functions $v_r(x) = x^{2r}$, and neglet the error term in (12). For $r = 0, \ldots, k-1$ define $f_r(x) = v_r(x)\log(1-\cos(x)))$. Now find the solution $\mathbf{c}^k_h = (c_{0,h}, \ldots, c_{k-1,h})$ of the resulting linear system of k equations

$$J(v_r) = T^n_{0,\beta^m}(f_r) + L^n_{\mathbf{c}^k_h}(v_r), \quad r = 1, \ldots, k. \quad (14)$$

Such solution $\mathbf{c}^k_h$ approximates the vector $\mathbf{c}^k$ of correction coefficients. In the above system of equations it is necessary to use a high value of the number $(m-1)/2$ of coefficients for boundary correction (say 20) in order to obtain the logarithm coefficients with at least 16 digits of precision. In practice setting $h < 1/40$ we obtained that $\mathbf{c}^k_h$ and $\mathbf{c}^k$ agree in at least 16 digits for several values of the number k of correction coefficients (k=1,2,...,23). Table 1 shows the numerical values with 16 digits of accuracy of the correction coefficents for several values of k yielding quadrature rules of orders up to 47.

$k = 1$, order 3	$k = 9$, order 19	$k = 23$, order 47
-4.368901313378636e0	-4.160034254640938e0	-4.145923335627446e0
	-1.255784908320719e-1	-1.386416515467072e-1
	2.659178193871165e-2	3.696816558728432e-2
$k = 2$, order 5	-6.793357704929117e-3	-1.389296673957712e-2
-4.247107485145063d0	1.626249096064179e-3	5.841334399889346e-3
-6.089691411678654d-2	-3.236208747595177e-4	-2.520528122470227e-3
	4.844335303175164e-5	1.069517295333890e-3
	-4.762800065295215e-6	-4.352385471826538e-4
$k = 4$, order 9	2.284551690365669e-7	1.670483827307765e-4
-4.190051589455464e0		-5.971537614730036e-5
-1.004861468415972e-1		1.967563865292637e-5
1.199246623905805e-2	$k = 11$, order 23	-5.918760116133687e-6
-9.311813590468452e-4	-4.155783090908638e0	1.610231184772598e-6
	-1.294218950761994e-1	-3.922351762206741e-7
	2.942643249138912e-2	8.458951628227212e-8
$k = 7$ order 15	-8.488627142045365e-3	-1.593821007821688e-8
-4.166775472248396e0	2.439492182527228e-3	2.581241878549816e-9
-1.196390890640811e-1	-6.312309842672700e-4	-3.518577833024770e-10
2.254506318892512e-2	1.378160130913916e-4	3.923937188781130e-11
-4.686840648506539e-3	-2.391312672959715e-5	-3.436481137272402e-12
8.073243691191345e-4	3.058919640099404e-6	2.215642935271013e-13
-9.490190027441715e-5	-2.548463452057683e-7	-9.348460581901533e-15
5.523489697421589e-6	1.033393966259407e-8	1.936111774897271e-16

Table 1: Correction coefficients $\mathbf{c}^k$ for $k = 1, 2, 4, 7, 9, 11, 23$.

4 Numerical tests

In this section we test the performance of the quadrature rules of the type (13) where the function v has period 2π. On all tables shown $n+1$ is the number of sampling points on the interval $[-\pi, \pi]$.

Example 1: Table 2 shows the results of the accuracy of the quadratures to approximate $\int_{-\pi}^{\pi} e^{2\cos(2x)+\sin(3x)} \log(\sqrt{2}(1-\cos(x)))dx$.

n	Relative Error, 23 correction coefficients
60	9.3×10^{-11}
70	3.1×10^{-12}
80	5.3×10^{-14}
90	5.4×10^{-16}

Table 2: Accuracy of the quadrature (13) to approximate the integral of Example 1 with 23 correction coefficients.

Example 2: Approximate $\displaystyle\int_{-\pi}^{\pi} e^{2\cos(8x)+\sin(9x)} \log(\sqrt{2}(1-\cos(x)))dx.$

n	Relative Error, 23 correction coefficients
100	1.2×10^{-5}
150	3.6×10^{-9}
200	8.3×10^{-11}
250	3.0×10^{-13}
280	4.5×10^{-15}

Table 3: Accuracy of the quadrature (13) to approximate the integral of Example 2 with 23 correction coefficients.

4.1 Calculation of convolutions

We describe now how to use quadratures of the type (13) to approximate a convolution of the form

$$g(t) = \int_0^{2\pi} v(\theta)\log(\omega(1-\cos(t-\theta)))d\theta \text{ for } t \in [0, 2\pi]. \tag{15}$$

Let n be an even positive integer. Define $h = 2\pi/n$, and let $t_j = \theta_j = -\pi + jh$ for any integer j. Let $v_j = v(\theta_j)$, and $z_j = \log(\omega(1-\cos(\theta_j)))$. Then

$$\begin{aligned} g(t_q) &\approx h \sum_{p=0, p\neq q}^{n-1} v_p z_{q-p} + h(\log(\omega h^2) + c_0)v_q + h\sum_{r=1}^{k-1} c_r(v_{q+r} + v_{q-r}) \\ &= h\sum_{p=0}^{n-1} v_p \tilde{z}_{q-p}, \end{aligned}$$

where $\tilde{z}$ is defined as follows: $\tilde{z}_{n/2} = \log(\omega h^2) + c_0$, $\tilde{z}_{n/2+j} = z_{n/2+j} + c_j$, and $\tilde{z}_{n/2-j} = z_{n/2-j} + c_j$, for $j = 1, ..., k-1$ provided $n \geq 2k$. We extend $\tilde{z}_j$ to all integers j as : $\tilde{z}_{nm+p} = \tilde{z}_p$ for all integer m, and all integer $p \in$

$[0, n-1]$. In this way we have that $g(t_q) \approx h \sum_{p=0}^{n-1} v_p \tilde{z}_{q-p}$ with an approximation error proportional to h^{2k+1}. The previous periodic discrete convolution can be calculated efficiently by means of FFT in $O(n\log(n))$ arithmetic operations.

Example 3: The following convolution appears in direct acoustic obstacle scattering in $\mathbb{R}^2$ (see [3]): approximate $\int_{-\pi}^{\pi} v(\theta)\log(4\sin^2(\frac{t-\theta}{2}))d\theta$, $t \in [0, 2\pi]$, where $v(\theta) = e^{2\cos(8\theta)+\sin(9\theta)}$.

In this case $\log(4\sin^2(\frac{t-\theta}{2})) = \log(2(1-\cos(t-\theta)))$. Hence we take $\omega = 2$ in (15). Table 4 shows the numerical results.

n	Relative Error, 23 correction coefficients
200	2.4×10^{-11}
280	3.8×10^{-15}

Table 4: Accuracy of the quadrature (13) to approximate the convolution of Example 3 with 23 correction coefficients.

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Received: January 8, 2008