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Quadrature Formulas with Exponential Convergence and Calculation of the Fermi–Dirac Integrals

Corresponding Member of the RAS N. N. Kalitkin[a]* and S. A. Kolganov[b]

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Abstract—A class of functions for which the trapezoidal rule has superpower convergence is described: these are infinitely differentiable functions all of whose odd derivatives take equal values at the left and right endpoints of the integration interval. An heuristic law is revealed; namely, the convergence exponentially depends on the number of nodes, and the exponent equals the ratio of the length of integration interval to the distance from this interval to the nearest pole of the integrand. On the basis of the obtained formulas, a method for calculating the Fermi–Dirac integrals of half-integer order is proposed, which is substantially more economical than all known computational methods. As a byproduct, an asymptotics of the Bernoulli numbers is found.

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1. PROBLEM

We consider only the problem of evaluating integrals of functions $u(x)$ having continuous derivatives of arbitrarily high order on the integration interval (see, e.g., [1–3]). In practice, this problem is usually solved on a uniform (or reducible to uniform) grid $\omega_N = \{x_n, n = 0, \ldots, N\}$ by using the simplest quadratures, such as the trapezoidal rule, the quadratic mean formula, Simpson's rule, etc. The error of such a formula is estimated as $\delta < \mathrm{const} \cdot M_p \cdot h^p = O(h^p) = O(N^{-p})$, where p is the accuracy order of the formula $M_p = \max|u^{(p)}(x)|$. This is a power convergence. It is fairly slow, and high accuracy is achieved only at large N. Such quadratures are rather computationally intensive.

The convergence of the Gauss–Christoffel quadrature is much more rapid. For example, the error of the classical Gaussian quadrature for integration over the interval $[-1, 1]$ with weight $\rho(x) = 1$ can be estimated (after simplifying the factorial multipliers) as

$$\delta \prec \sqrt{\frac{\pi}{N}} \frac{b-a}{4} \left(e\frac{b-a}{8N}\right)^{2N} M_{2N}. \quad (1)$$

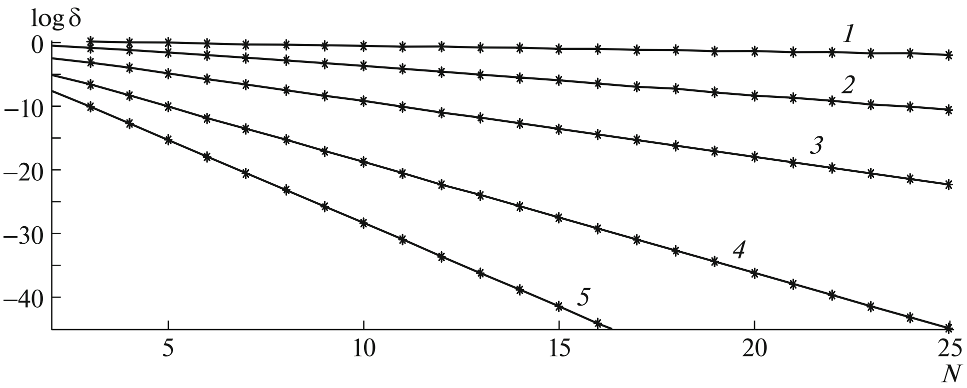
The Hermite quadrature for integration over the interval $[-1, 1]$ with weight $\rho(x) = (1-x^2)^{-1/2}$ has error

$$\delta \le \sqrt{\frac{\pi}{N}} \left(\frac{e}{2\sqrt{2}N}\right)^{2N} M_{2N}. \quad (2)$$

Formulas (1) and (2) can be written (up to logarithmically small terms) in the form $\delta \sim \alpha \cdot \exp(-\beta N)$ therefore, such convergence is close to exponential. The computational complexity of similar formulas is immeasurably lower than that of quadratures with power convergence. However, the nodes and weight of the Gauss–Christoffel quadrature have been found only for certain intervals and integration weights $\rho(x)$. Moreover, these weights and nodes can be calculated by simple formulas for any N only in the case of Hermite quadratures. For other quadratures, nodes and weights can be evaluated exactly (in radicals) only for $N \le 3$ or $N = 5$. This strongly restricts the application of such quadratures in practice.

In this paper, we show that if $u(x)$ can be extended beyond both boundaries of the interval to an even function, then the trapezoidal rule on a uniform grid convergences exponentially. Moreover, the coefficient β in the exponent is determined by the distance to the nearest pole in the complex plane. This opens up new possibilities for constructing quadratures of low complexity. We also give an example interesting for problems of quantum mechanics, namely, evaluate the Fermi–Dirac integrals of half-integer order. As a byproduct, we obtain an asymptotics of the Bernoulli numbers.

[a] Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Moscow, 125047 Russia
[b] National Research University of Electronic Technology (MIET), Zelenograd, Moscow, 124498 Russia
* e-mail: kalitkin@imamod.ru



The error of the trapezoidal quadrature for (5) at $r = 0$ and $q = 1$. The figures near the lines correspond to various values of c (*1*, 1.10; *2*, 1.75; *3*, 2.72; *4*, 7.39; *5*, 20.09).

2. THE CASE OF EXPONENTIAL CONVERGENCE

Suppose that the derivatives $u^{(p)}(x)$ exist and are continuous on $[a;b]$ for any p It is required to evaluate the integral

$$U = \int_a^b u(x)dx. \tag{3}$$

We introduce the uniform grid ω_N with $x_0 = a$ and $x_N = b$ and apply the Euler–Maclaurin formula [4]

$$\begin{aligned} U_N &= h\left(\frac{u_0}{2} + u_1 + u_2 + \ldots + u_{N-1} + \frac{u_N}{2}\right) \\ &+\sum_{p=1} (-1)^p a_p h^{2p}(u_N^{(2p-1)} - u_0^{(2p-1)}), \quad a_p \sim M_{2p-1}, \end{aligned} \tag{4}$$

which is based on the trapezoidal rule. If this sum is cut off after the Pth term, then the first discarded term is residual. Its value is $\delta_P \sim O(h^{2P+2})$. In this case, quadrature (4) has power convergence.

Suppose that $u(x)$ is such that all of its odd derivatives take equal values at the right and left endpoints: $u^{(2p-1)}(a) = u^{(2p-1)}(b)$. Then the sum in (4) vanishes. The remaining part of the quadrature is simply the trapezoidal rule. This implies the following assertions.

Statement. *If $u^{(2p-1)}(a) = u^{(2p-1)}(b)$ for any p, then the trapezoidal rule converges on a uniform grid faster than any power.*

Special case. The above statement is valid, in particular, if $u(x)$ extends beyond both endpoints of the interval to an even function:

$$u^{(2p-1)}(a) = u^{(2p-1)}(b) = 0.$$

Thus, we have determined a class of functions for which the trapezoidal rule has superpower convergence. It remains to find the law of this convergence. We shall obtain such a law heuristically for the test example

$$U(r,q) = \int_0^\pi \frac{(c^2-1)\cdot c^r \cos(rx)}{(c^2 - 2c\cos x + 1)^q}dx, \quad c > 1. \tag{5}$$

The integrand has poles of order q at the points

$$x^* = 2\pi m \pm i\ln(c), \quad -\infty < m < +\infty. \tag{6}$$

On the integration interval $[0;\pi]$, the derivatives $u^{(p)}(x)$ of any orders exist and are continuous, and at its endpoints, the evenness conditions are satisfies. For $q = 1$, the exact value of integral (5) is known: $U(r,1) = \pi$.

Figure shows the results of computing the test integral (5) for $q = 1, r = 0$, and various c. Computation was performed with the enhanced digit capacity of 45 decimal digits. The error δ_N was calculated directly from the known exact value. We see that the dependence of $\ln \delta_N$ on N turns out to be linear. This is evidence for the exponential convergence of the trapezoidal rule for such a function.

We see that, even for few nodes, very high accuracy is achieved. This demonstrates the practical importance of the method.

The slopes of the straight lines in the figure depend on c; moreover, the error is well described by the relation

$$\ln\delta_N = \alpha - \beta N, \quad \beta = \text{const}\ln c. \tag{7}$$

It is easy to see that the slope β equals the length between points of the integration interval and the nearest pole (6). Note that this ratio, unlike the error estimates of the Gauss–Christoffel quadrature, in no way involves the norms of the derivatives of $u(x)$.

The same results (but with a slower rectification of the lines) were obtained for $r = 1, 2, \ldots$, as well as for the case $q = 2$ of a double pole. Thus, the obtained heuristic laws are of the same character.

Remark. The convergence obtained above is purely exponential. This makes it possible to construct a posteriori asymptotically exact error estimates on the basis of computations for two different N, by analogy with Richardson's method for power convergence. The convergence of the Gauss–Christoffel quadrature is even somewhat faster than the exponential rate [1, 2], but a posteriori error estimates for it cannot be obtained from computations with different N. Therefore, for computations with guaranteed accuracy, the method proposed above is more convenient than the Gauss–Christoffel method.

3. COMPUTATION OF THE FERMI–DIRAC INTEGRALS OF HALF-INTEGER ORDER

The Fermi–Dirac integrals arise in problems of quantum mechanics. These are the angular momenta for the Fermian distribution. They are defined as [5]

$$I_k(x) = \int\limits_0^\infty \frac{t^k}{1+e^{t-x}}dt, \quad k > -1, \quad -\infty < x < +\infty. \quad (8)$$

In quantum mechanics, only integer and half-integer values of k are used. For integer k, the problem of computation with 17 decimal digits was solved in [6]. Half-integer orders k have been extensively studied, and methods for evaluating Fermi–Dirac integrals of such orders with 15 decimal digits have been suggested; however, these methods are not economical enough. In what follows, we propose an efficient method for computing the corresponding quadratures (8).

The integrand in (8) with $t = 0$ and half-integer k has a singular point, and the integration interval is infinite. We overcome both difficulties by making the change of variables $t = \gamma\xi^2(1-\xi^2)^{-1}, 0 \le \xi \le 1$, $\gamma =$ const > 0. It reduces (8) to the form

$$I_k(x) = \int\limits_0^1 \frac{2\gamma^{k+1}\xi^{2k+1}d\xi}{\{1+\exp[\gamma\xi^2(1-\xi^2)^{-1}-x]\}(1-\xi^2)^{k+2}}, \quad (9)$$
$$k = -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots.$$

For half-integer k, the exponent of t in the numerator is even. The odd derivatives of the integrand with respect to ξ vanish at both endpoints: at $\xi = 0$, by virtue of evenness, and at $\xi = 1$, due to the exponential in the denominator. Therefore, (9) satisfies the requirements in Section 2, and the trapezoidal rule on a uniform grid ensures exponential convergence.

We choose the constant γ so that the maximum of the integrand is attained at $\xi = \frac{1}{2}$. This gives

$$1+\exp\left(x-\frac{\gamma}{3}\right) = \frac{\gamma}{3\left(k+\frac{7}{8}\right)}. \quad (10)$$

The root $\gamma(x)$ of Eq. (10) is easy to compute for each x by Newton's method.

The trapezoidal quadrature for (9) with γ satisfying (10) is the fastest algorithm for directly computing $I_k(x)$ with half-integer k. To obtain 16 decimal digits for $x < 0$, it suffices to take the grid with $N = 32$. As x increases, the number of nodes grows, but even for $x = 50$ and $k = \frac{7}{2}$, as few as 1024 nodes are sufficient. This is much more economical than all quadratures known previously.

3.1. Convergence

The poles of integrand (9) form sequences converging to the points $\xi = \pm 1$. The point $\xi = 1$ is an endpoint of the integration interval. This does not fit the heuristic law governing the rate of convergence, which was described in Section 2. The reason for this is that the case under consideration is much more complicated: all derivatives tend to zero very rapidly as $\xi \to +1$ because of the exponential in the denominator. Therefore, the convergence remains exponential, although estimating its coefficient requires a more thorough study.

4. ASYMPTOTICS OF THE BERNOULLI NUMBERS

In the course of the present research, we obtained an interesting result. For $x > 0$, the Fermi–Dirac functions admit an asymptotic expansion in powers of x^{-2} The coefficients of this expansion are expressed in terms of the Bernoulli numbers. We have obtained a heuristic asymptotics of these coefficients for large indices. An exact expression for the Bernoulli numbers indices. An exact expression for:

$$B_{2m} = (-1)^{m-1}\frac{(2m)!}{\pi^{2m}2^{2m-1}}A_n, \quad A_n = \sum_{p-1}^{\infty}\frac{1}{p^{2m}}. \quad (11)$$

This expression is convenient for calculating Bernoulli numbers with large indices, because $A_n \to 1$ if $n \to \infty$. Expression (11) was obtained for even Bernoulli coefficients; we remind, however, that all odd coefficients, except B_1.

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