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Filon–Clenshaw–Curtis rules for a class of highly-oscillatory integrals with logarithmic singularities

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ABSTRACT

In this work we propose and analyse a numerical method for computing a family of highly oscillatory integrals with logarithmic singularities. For these quadrature rules we derive error estimates in terms of N, the number of nodes, k the rate of oscillations and a Sobolev-like regularity of the function. We prove that the method is not only robust but the error even decreases, for fixed N, as k increases. Practical issues about the implementation of the rule are also covered in this paper by: (a) writing down ready-to-implement algorithms; (b) analysing the numerical stability of the computations and (c) estimating the overall computational cost. We finish by showing some numerical experiments which illustrate the theoretical results presented in this paper.

1. Introduction

This paper concerns itself with the approximation of

$$\mathcal{I}_k^\alpha(f) := \int_{-1}^{1} f(x)\ \log((x-\alpha)^2)\ \exp(ikx)\,\mathrm{d}x \tag{1.1}$$

where $\alpha \in [-1, 1]$. For the sake of simplicity, we will assume throughout this paper that $k \geq 0$, although the algorithm and the theoretical results can be straightforwardly adapted for $k \leq 0$.

Our aim is to design numerical methods whose rates of convergence do not depend on k but only on f and the number of nodes of the quadrature rules. No information about the derivatives, which is very common in the approximation of oscillatory integrals (see [1] or [2] and references therein), will be used, which results in a simpler and less restrictive method. At first sight, $\alpha \in \{-1, 0, 1\}$ could be the more common cases but since the analysis we develop here is actually valid for any $\alpha \in [-1, 1]$, we cover the general case in this paper.

We choose in this work the Clenshaw–Curtis approach:

$$\mathcal{I}_{k,N}^\alpha(f) := \int_{-1}^{1} \mathcal{Q}_N f(x)\ \log((x-\alpha)^2)\ \exp(ikx)\,\mathrm{d}x \approx \mathcal{I}_k^\alpha(f), \tag{1.2}$$

where

$$\mathbb{P}_N \ni \mathcal{Q}_N f, \quad \text{s.t. } \big(\mathcal{Q}_N f\big)(\cos(n\pi/N)) = f(\cos(n\pi/N)),\ n = 0, \ldots, N. \tag{1.3}$$

In other words, $\mathcal{Q}_N f$ is the polynomial of degree N which interpolates f at Chebyshev nodes.

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Classical, and modified, Clenshaw–Curtis rules (1.2) enjoy very good properties which have made them very popular in the scientific literature (cf. [3–7]) and have been considered competitive with respect to Gaussian rules even for smooth integrands (we refer to [8] for an interesting discussion about this fact). First of all, the error of the rule is, in the worst case, like the error of the interpolating polynomial in $L_1(-1, 1)$. Thus, the rule is robust with respect to k and it inherits the excellent approximation properties of the interpolant. On the other hand, and from a more practical view, nested grids can be used in the computations. Hence, if $\mathcal{I}_{k,N}(f)$ has been already computed, $\mathcal{I}_{k,2N}(f)$ only requires N new evaluations of f, i.e. previous calculations can be reused. Moreover, by comparing both approximations, a-posteriori error estimate is at our disposal almost for free. Finally, $\mathcal{Q}_N f$ can be expressed in the Chebyshev basis very fast, in about $\mathcal{O}(N \log N)$ operations, using FFT techniques.

If $k = 0$, or if k is small enough ($k \le 2$ has been used throughout this paper), the complex exponential can be incorporated to the definition of f. This leads us to consider, in the same spirit, the following integral and numerical approximation,

$$\mathcal{I}_0^\alpha(f) := \int_{-1}^{1} f(x)\ \log((x-\alpha)^2)\,\mathrm{d}x \approx \int_{-1}^{1} \mathcal{Q}_N f(x)\ \log((x-\alpha)^2)\,\mathrm{d}x =: \mathcal{I}_{0,N}^\alpha(f). \tag{1.4}$$

This problem is also dealt with in this work since the combination of both algorithms gives rise to a method which can be applied to non-, mildly and highly oscillatory integrals.

For these rule we will show that the rule converges superalgebraically for smooth functions f. Moreover, the error is not only not deteriorated as k increases but it even decreases as k^{-1} as $k \to \infty$. Furthermore, for some particular values of α, which include the more common choices $\alpha \in \{-1, 0, 1\}$, the error decay faster, as k^{-2}, which means that both, the absolute and relative error of the rule decreases (cf. Theorem 2.4).

The implementation of the rule hinges on finding a way to compute, fast and accurately, the weights

$$\xi_n^\alpha(k) := \int_{-1}^{1} T_n(x) \log((x-\alpha)^2)\ \exp(ikx)\,\mathrm{d}x, \quad k > 2, \tag{1.5}$$

$$\xi_n^\alpha := \xi_n^\alpha(0) = \int_{-1}^{1} T_n(x)\ \log((x-\alpha)^2)\,\mathrm{d}x \tag{1.6}$$

($T_n(x) := \cos(n \arccos x)$ is the Chebyshev polynomial of the first kind) for $n = 0, 1, \ldots, N$. The second set of coefficients $(\xi_n^\alpha)_n$ is computed by using a three-term recurrence relation which we show to be stable. For the first set, $(\xi_n^\alpha(k))_n$, the situation is more delicate. First we derive a new three-term linear recurrence which can be used to evaluate $\xi_n^\alpha(k)$. The calculations, however, turn out to be stable only for $n \le k$. This could be understood, somehow, as consequence of potentially handling two different sources of oscillations in $\xi_n^\alpha(k)$. The most obvious is that coming from the complex exponential, which is fixed independent of n. However, when n is large, the Chebyshev polynomials, like the classical orthogonal polynomials, have all their roots in $[-1, 1]$. This results in a increasing oscillatory behaviour of the polynomial as $n \to \infty$. As long as the first oscillations source dominates the second one, i.e. as $k > n$, the recurrence is stable: any perturbation introduced in the computation is amplified very little. However, when $n > k$ increases, such perturbations are hugely magnified, which makes this approach completely useless. Of course, if k is large, so should be N to find these instabilities. Hence, this only causes difficulties for practical computations in the middle range, that is, when k is not yet very large but we need to use a relatively large number of points to evaluate the integral within the prescribed precision.

This phenomenon is not new: It has been already observed, among other examples, when computing the simpler integral

$$\int_{-1}^{1} T_n(x) \exp(ikx)\,\mathrm{d}x.$$

(See [9] and references therein.) Actually, the problem is circumvented using the same idea, the so-called Oliver method (cf. [10]) which consists in rewriting appropriately the difference equation used before now as a tridiagonal linear system whose (unique) solution gives the sought coefficients except the last one which is part now of the right-hand-side. Therefore, the evaluation of this last coefficient has to be carried out in a different way. Thus, we make use of an asymptotic argument, namely the Jacobi–Anger expansion, which expresses $\xi_N^\alpha(k)$ as a series whose terms are a product of Bessel functions and integrals as in (1.6). Despite the fact that it could seem at first sight, the series can also be summed in about $\mathcal{O}(N)$ operations. The resulting algorithm has a cost $\mathcal{O}(N \log N)$, cost which is lead by the FFT method used in the construction of the interpolant $\mathcal{Q}_N f$.

Let us point out that the case of $\alpha = 0$, for both the oscillatory and non-oscillatory case, has been previously considered in [11] using a different strategy. Roughly speaking, it relies on using the asymptotic Jacobi–Anger expansion for all the coefficients, no matter how large k is respect to n. Our approach is, in our opinion, more optimal since the algorithm is simpler to implement and the computational cost is smaller.

The interest in designing efficient methods for approximating oscillatory integrals has been increased in the last years, fuelled by new problems like high frequency scattering simulations (cf. [11,12,9]). For instance, in the boundary integral method, the assembly of the matrix of the systems requires computing highly oscillatory integrals which are smooth except on the diagonal. Hence, after appropriate change of variables, we can reduce the problem to evaluate

$$\int_0^1 f(s) \exp(iks)\,\mathrm{d}s.$$