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Gauss rules associated with nearly singular weights

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A R T I C L E I N F O

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A B S T R A C T

We consider the problem of evaluating $\int_{-1}^{1} f(x)G(x)(1-x^2)^{-1/2}dx$, when f is smooth and G is nearly singular and non-negative. For this we construct a Gauss quadrature formula w.r.t. the weight $G(x)(1-x^2)^{-1/2}$. Once the factor G has been chosen, the procedure is relatively simple and mainly involves the application of *FFT* to compute a finite number of coefficients of the Chebyshev series expansion of G which in turn are used to calculate modified moments.

It is shown that this approach is very effective when the complexity of f is high, or when f is parametric and the integral must be calculated for many values of the parameters. For this, there is presented a selection of numerical examples which allows comparison with other methods. In particular, there is considered the evaluation of Hadamard finite part integrals when the regular part of the integrand is nearly singular.

1. Introduction

Over the last decades a great variety of boundary problems have been reformulated as boundary integral equations involving nearly singular and strongly singular integrals which cannot be computed accurately using ordinary quadrature rules. Some of these problems have been established in terms of multiple integrals whose study can be carried out by considering the one-dimensional case (cf. [1,2,14,18]). The latter is the issue to which we refer in this article. For convenience and without loss of generality, in what follows all integrals are defined over the interval $[-1, 1]$.

Let $I_W(F) = \int_{-1}^{1} F(x)W(x)\,dx$, where F is the integrand and W is a weight function. It is most likely that $I_W(p)$ is used to approximate $I_W(F)$, where p is the polynomial of degree $n-1$, that interpolates F at n distinct points of $[-1, 1]$. Once the corresponding quadrature formula has been calculated, the weight W is usually fixed, whereas F varies freely in a given class. Unfortunately, in many cases, F has a nature that does not favor the use of digital resources. This phenomenon manifests when F has a meromorphic component having *difficult poles*, i.e. poles located very close to $[-1, 1]$, or when the scale of F is influenced by a factor that varies exponentially (cf. [22]). In cases like these, it is commonly said that F is nearly singular, but here we also say that F is a *difficult function*. The adjective *smooth* is used when referring to functions that are considered as non-difficult.[2]

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[2] The term “difficult” was used by W. Gautschi to describe the poles of the integrand which are located near the interval of integration.

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If F shows difficult behavior, then the following step is to write F as the product of two factors, say $F = fG$, where f is no longer difficult, and G is a non-negative function. Thus, f is now integrated w.r.t. GW. If the issue is due to algebraic singularities of the integrand, e.g. when F is meromorphic on a neighborhood of $[-1, 1]$, then one can select $f = q_0 F$ and $G = 1/q_0$, where q_0 is a polynomial whose zeros coincide with *difficult poles* of F. This approach based on rational functions has been studied by many authors, among whom W. Gautschi is probably the most cited (see, for example, [7–13,22]). In addition to Gautschi's work, different techniques have been developed to handle difficult poles (cf. [6,13]). As far we know, all these methods are often costly, because they depend largely on features of the integrand and, in most cases, expert judgment is needed.

If f is meromorphic and G is poorly scaled but not related to difficult poles, then it is indicated the use of Gauss formulas for weights of the form GW/q_0. This hint appears without any technical treatment in [11]. On the other hand, following the ideas of Clenshaw and Curtis [5], it has been shown recently that the coefficients of the interpolatory quadrature formula w.r.t. GW, can be calculated with great precision when G is replaced by its Chebyshev series expansion (cf. [3]). Despite [11], we are only interested in examine the case in which $q_0 \equiv 1$ and G can also possess difficult poles, if any. The reason for this is to avoid the calculation of residues, a problem which is often ill conditioned.

The goal of this paper is to present a method to evaluate efficiently the integral $I_{GW}(f)$, when W is the Chebyshev weight function of the first kind and G is nearly singular. For this, we show how to calculate accurately nodes and coefficients of the Gauss quadrature formula associated with GW. The calculation process is mainly based on using the modified Chebyshev method and Fast Fourier Transform (*FFT*). As a consequence, we can integrate a wide variety of difficult functions, at a cost that may be relatively low when either the complexity of f is high or f depends on some parameters.

The remainder of this article is organized as follows.

Section 2 describes the implementation of this approach, in particular, the calculation of modified moments. Some numerical examples are listed in Section 3 in order to verify the accuracy of the proposed method, and also to complement the explanation given in the previous section.

Sections 4 and 5 show some cases in which our approach is particularly effective. Section 4 suggests how to choose the weight function to evaluate Hadamard finite-part integrals, while the main target of Section 5 is the analysis of complexity. Some concluding remarks are given in Section 6.

2. Description of the numerical procedure

2.1. Preliminaries and statement of the quadrature formula

Let $\omega(x)$ be a nonnegative function on the real interval $[c, d]$, such that all moments $M_\nu = \int_c^d x^\nu \omega(x)dx$, $\nu = 0, 1, 2, \ldots$, are finite and $M_0 > 0$. Let Π be the space of real polynomials and Π_n the subspace of polynomials of degree $\leq n$. The inner product associated with ω is defined as

$$\langle P_1, P_2\rangle_\omega = \int_c^d P_1(x)P_2(x)\omega(x)dx, \quad P_1, P_2 \in \Pi.$$

Suppose that this inner product is positive definite on Π, i.e. $\|P\|^2 = \langle P, P\rangle_\omega > 0$ for all $P \in \Pi$.

Let $Q_k = x^k + \delta_{k-1}x^{k-1} + \cdots \in \Pi_k$, $k = 0, 1, 2, \ldots$. These polynomials Q_k are called (monic) orthogonal polynomials w.r.t. ω if $\langle Q_k, Q_l\rangle_\omega = 0$ for $k \neq l$, and $\|Q_k\| > 0$, $k = 0, 1, \ldots$.

Orthogonal polynomials and numerical integration are two closely interrelated topics. In effect, the integral $I_\omega(f) = \int_c^d f(x)\omega(x)dx$ can be approximated by a finite sum $S_n(f) = \sum_{k=1}^n \lambda_{n,k} f(x_{n,k})$, such that $I_\omega(P) = S_n(P)$, for all $P \in \Pi_{2n-1}$. The approximation formula $I_\omega(f) \approx S_n(f)$ is the n-point Gauss quadrature rule associated with ω, whose nodes $\{x_{n,k}\}$ are the n distinct zeros of the nth orthogonal polynomial Q_n. Moreover, for all $k \in \{1, \ldots, n\}$, it holds that $\lambda_{n,k} > 0$ and $-1 < x_{n,k} < 1$.

One of the most important properties is that $\{Q_k\}$ satisfies a three term recurrence relation

$$Q_{k+1}(x) = (x - a_k)Q_k(x) - b_k Q_{k-1}(x), \tag{1}$$

with $Q_0 \equiv 1$, $Q_{-1} \equiv 0$, and $b_k > 0$, $k = 1, \ldots, n$.

The typical procedure to calculate $S_n(f)$ uses (1) to construct the Jacobi matrix associated with the weight function ω (see [11])

$$J_\infty(\omega) = \begin{pmatrix} a_0 & \sqrt{b_1} & & & 0 \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \sqrt{b_2} & a_2 & \sqrt{b_3} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{pmatrix}.$$