Gauss rules associated with nearly singular weights

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Abstract

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, it is presented a selection of numerical examples which allows comparison with other methods. In particular, it is considered the evaluation of Hadamard finite part integrals when the regular part of the integrand is nearly singular.

Keywords: Gauss quadrature formula, rational quadrature formula, difficult pole, Chebyshev series method, nearly singular integral.

2010 MSC: 65D32, 41A55

1. Introduction

Over the last decades a great variety of boundary problems have been re-formulated as boundary integral equations involving nearly singular and

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\textsuperscript{1}These authors were supported by Ministerio de Ciencia e Innovación, Spain, under grant number MTM2011-22713.
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.\(^2\)

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 \(f = q_0F\) 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

\(^2\)The term “difficult” was used by W. Gautschi to describe the poles of the integrand which are located near the interval of integration.
shown recently that the coefficients of the interpolatory quadrature formula w.r.t. \( G_W \), 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.

Section 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 \( \Pi \) be the space of real polynomials and \( \Pi_n \) the subspace of polynomials of degree \( \leq n \). The inner product associated with \( \omega \) 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 \( \Pi \), i.e. \( \|P\|^2 = \langle P, P \rangle_\omega > 0 \) for all \( P \in \Pi \).
Let \( Q_k = x^k + \delta_k x^{k-1} + \cdots \in \Pi_k, k = 0, 1, 2, \cdots \). These polynomials \( Q_k \) are called (monic) orthogonal polynomials w.r.t. \( \omega \) if \( \langle Q_k, Q_l \rangle_\omega = 0 \) for \( k \neq l \), and \( \|Q_k\| > 0, k = 0, 1, \cdots \)

Orthogonal polynomials and numerical integration are two closely inter-related topics. In effect, the integral \( I_\omega(f) = \int f(x)\omega(x)dx \) 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 \( \omega \), whose nodes \( \{x_{n,k}\} \) are the \( n \) distinct zeros of the \( n \)th orthogonal polynomial \( Q_n \). Moreover, for all \( k \in \{1, \cdots, n\} \), 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

\[
Q_{k+1}(x) = (x - a_k)Q_k(x) - b_kQ_{k-1}(x),
\]
with \( Q_0 \equiv 1, Q_{-1} \equiv 0 \), and \( b_k > 0, k = 1, \cdots, n \).

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

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

Let \( J_n \) be the \( n \times n \) leading principal minor matrix of \( J_\infty \). If \( J_n = VDV^t \), where \( D \) is diagonal, and \( C_k \) is the \( k \)th column of the orthogonal matrix \( V \), then the eigenvalues of \( J_n \) coincide with the \( n \) zeros of \( Q_n \), and \( \lambda_{n,k} = b_0 C_k(1)^2, k = 1, \cdots, n \), with \( b_0 = \int_{-1}^1 \omega(x)dx \).

The following is the well known \( N \)-point Gauss-Chebyshev (GC) quadrature formula associated with the Chebyshev weight function of the first kind \( \omega(x) = (1 - x^2)^{-1/2} \).

\[
\int_{-1}^1 f(x)G(x) \frac{dx}{\sqrt{1-x^2}} = \sum_{j=1}^N \Lambda_{N,j} f(\tau_{N,j})G(\tau_{N,j}) + \mathcal{E}^{GC}_N(fG),
\]
where \( \mathcal{E}^{GC}_N(fG) \) is the remainder, \( \tau_{N,k} = \cos((2k-1)\pi/2N) \), and \( \Lambda_{N,k} = \pi/N, k = 1, \cdots, N \).
The mathematical formulation of the above parameters is so simple that one can increase $N$ up to very large values without losing precision.

The corresponding orthogonal polynomials are the (nonmonic) Chebyshev polynomials of the first kind: $T_N(x) = 2^{N-1}x^N + \cdots$, which satisfy the following relation

$$T_{N+1}(x) = 2xT_N(x) - T_{N-1}(x), \quad N = 1, 2, \cdots, \quad (3)$$

$T_0 \equiv 1$, and $T_{-1} \equiv 0$.

Suppose that $G(x)$ is a function non-negative on $[-1,1]$. The Gauss quadrature formula we want to implement is that associated with the weight function $GW$, where $W(x) = p(x)/(\pi \sqrt{1 - x^2})$, and $p$ is a polynomial non-negative on $[-1,1]$. It is defined as follows.

$$\int_{-1}^{1} f(x)G(x)W(x)dx = \sum_{j=1}^{n} \lambda_{n,j}f(x_{n,j}) + E_n^{MG}(f), \quad (4)$$

where $E_n^{MG}(f)$ is the quadrature error, the weights are given by

$$\lambda_{n,j} = \int_{-1}^{1} \frac{Q_n(x)}{Q'_n(x_{n,j})(x - x_{n,j})} G(x)W(x)dx, \quad j = 1, \cdots, n,$$

and $Q_n(x) = \prod_{j=1}^{n}(x - x_{n,j})$ is the $n$th monic orthogonal polynomial associated with the weight function $G(x)W(x)$.

### 2.2. Modified Chebyshev algorithm

Our immediate problem is to calculate the quadrature nodes $x_{n,j}$ and the coefficients $\lambda_{n,j}$ of formula (4). For this we are going to compute the coefficients $\{a_k, b_k\}$ of the recurrence relation (1) using the method proposed by Sack & Donovan [21] under conditions in which it is numerically stable (cf. [7, 11, 15]). Thus, we need to select a suitable sequence of polynomials $\{P_m\}$ satisfying a known recurrence relation. A wise decision is to define $P_m = T_m/2^{m-1}$, $m \geq 1$, and $P_0 = 1$. It follows from (3) that $\{P_m\}$ is generated recursively by

$$P_m(x) = xP_{m-1}(x) - 0.25P_{m-2}(x), \quad m \geq 3, \quad (5)$$

with the initial conditions $P_2(x) = x^2 - 0.5$, $P_1(x) = x$ and $P_0(x) = 1$. 

5
The mixed moments are given by \( \mu_{m,k} = \int_{-1}^{1} Q_k P_m GW \, dx \). Because of orthogonality, it holds that \( \mu_{m,k} = 0 \), provided \( m < k \).

From (1–5), we derive the following 2D-formula for \{\mu_{m,k}\}.

\[
\mu_{m,k+1} = \mu_{m+1,k} + 0.25\mu_{m-1,k} - a_k \mu_{m,k} - b_k \mu_{m-1,k},
\]

(6)

\( k = 0, 1, \ldots; m = 2, \ldots \)

The starting point of this procedure is the calculation of the modified moments \( \mu_{m,0}, m = 0, 1, \ldots, 2n - 1 \). The following steps are performed using (6) and must provide an estimate of the coefficients \{\(a_k, b_k\}\).

If \( m = 1 \) and \( k = 0 \), then \( \mu_{1,1} = \mu_{2,0} + 0.5\mu_{0,0} - a_0\mu_{1,0} \). Moreover, \( \mu_{0,0} = \int_{-1}^{1} GW \, dx \neq 0 \) and \( \mu_{m,-1} = 0 \).

From (6) and the orthogonality properties of \( Q_k \), and also considering the particular values \( m = k - 1, k \), we obtain the following system of linear equations with unknowns \( a_k \) and \( b_k \), \( k \geq 1 \).

\[
\begin{align*}
    a_k \mu_{k,k} + b_k \mu_{k,k-1} &= \mu_{k+1,k} \\
    b_k \mu_{k-1,k-1} &= \mu_{k,k},
\end{align*}
\]

with initial values \( a_0 = \mu_{1,0}\mu_{0,0}^{-1} \) and \( b_0 = \mu_{0,0} \).

Once we have estimated \( a_k \) and \( b_k \), \( k = 0, 1, \ldots, n - 1 \), we can construct the corresponding matrix \( J_n \).

2.3. Calculation of modified moments

The aim of this subsection is to calculate as accurately as possible the numbers

\[
\mu_{m,0} = \int_{-1}^{1} P_m(x) G(x)p(x) \, dx \sqrt{1-x^2}, \quad m = 0, 1, \ldots, 2n - 1.
\]

(7)

For this, it is sufficient the following partial sum of the Chebyshev series expansion of the function \( G \):

\[
S_{2n-1+d}(G) = \sum_{j=0}^{2n-1+d} A_j T_j,
\]

where the dash indicates that the first term in the sum is halved, \( d = \deg(p) \) and

\[
A_j = \frac{2}{\pi} \int_{-1}^{1} T_j(x) G(x) \frac{dx}{\sqrt{1-x^2}}; \quad j = 0, 1, \ldots, 2n - 1 + d.
\]
What we do here is to replace $G$ by $S_{2n-1+d}(G)$ into the integral (7).

There is a variety of results related to the convergence of $S_N(G)$, all linked to the nature of $G$. The following is the most important to us.

**Lemma 2.1.** Let $\omega(x) = (1 - x^2)^{-1/2}$, $-1 < x < 1$. If $G \in L_2([-1, 1], \omega)$, then $\lim_N \|G - S_N(G)\|_{2,\omega} = 0$.

**Proposition 2.1.** If $p = \sum_{k=0}^{d} \alpha_k T_k$, then

$$\mu_{m,0} = D_m \sum_{k=0}^{d} \alpha_k (A_{|k-m|} + A_{k+m}), \; m \geq 0,$$

where $D_m = 2^{-(m+1)}$, if $m \geq 1$, and $D_0 = 2^{-2}$.

In particular, if $p \equiv 1$, then

$$\mu_{m,0} = A_m / 2^m, \; m \geq 1, \; \mu_{0,0} = A_0 / 2.$$

**Proof.** Set $m \geq 1$. Lemma 2.1 says that the summation symbol can be extracted from the interior of the integral (7), i.e.

$$\mu_{m,0} = \frac{1}{2m-1} \sum_{k=0}^{d} \alpha_k \sum_{j=0}^{\infty} A_j \int_{-1}^{1} \frac{T_m(x)T_j(x)T_k(x)}{\pi \sqrt{1-x^2}} \; dx.$$

Using the equality $T_m T_k = (T_{m+k} + T_{m-k})/2$, we obtain that

$$\mu_{m,0} = \frac{1}{2^m} \sum_{j=0}^{\infty} A_j \sum_{k=0}^{d} \alpha_k \int_{-1}^{1} \frac{(T_{m+k}(x) + T_{m-k}(x))T_j(x)}{\pi \sqrt{1-x^2}} \; dx.$$

Equation (8) is derived from (10) and

$$\int_{-1}^{1} \frac{T_u(x)T_v(x)}{\sqrt{1-x^2}} \; dx = \begin{cases} \pi / 2 & \text{if } u = v \neq 0, \\ \pi & \text{if } u = v = 0, \\ 0 & \text{if } u \neq v. \end{cases}$$

If $m = 0$, then Eq. (8) also follows using orthogonality. \qed
2.4. Calculation of $A_j$

What is described below was used to develop a simple Matlab code to calculate $\{\tilde{A}_{j,N}\}_{j=0}^N$, where $\tilde{A}_{j,N}$ approximates $A_j$, being $N$ the number of points in the FFT function.

Let $\rho_{N,j} = e^{-j\pi/N}/N$. If $G$ is written as the sum of its even and odd parts, say $G = G_{\text{even}} + G_{\text{odd}}$. Then, the Chebyshev coefficients of $G_{\text{even}}$ are $A_{2j} \approx 2\Re(A_{j,N}^{(1)})$, where

$$A_{j,N}^{(1)} = \rho_{N,j} \sum_{k=0}^{N-1} G_{\text{even}}(\tau_{N,k}) \exp\left(-\frac{2k j \pi i}{N}\right), \quad (11)$$

and $A_0$ must be halved (cf. [3]).

Let $\psi_{N,k} = e^{-i\pi(2k+1)/(2N)}$. The coefficients $A_{2j+1}$ of $G_{\text{odd}}$ are approximated by $2\Re(A_{j,N}^{(2)})$, where

$$A_{j,N}^{(2)} = \rho_{N,j} \sum_{k=0}^{N-1} G_{\text{odd}}(\tau_{N,k}) \psi_{N,k} \exp\left(-\frac{2k j \pi i}{N}\right). \quad (12)$$

As before, $\{\tau_{N,k}\}_{k=1}^N$ stands for the zeros of the $N$th Chebyshev polynomial of the first kind, which proved to be more suitable than the equidistant ones. Here we should note that neither $\psi_{N,k}$ nor $\rho_{N,j}$ depend on $G$, therefore, they can be calculated just once and be used for several functions $G$. The structure of (11) and (12) allows to apply directly Matlab’s FFT function.

We expect that $\lim_{N} \tilde{A}_{j,N} = A_j$, for all $j$, but an experimental conclusion is that the error $R_{j,N} = |(\tilde{A}_{j,N} - A_j)/A_j|$ increases as $j$ becomes larger. Although no more than $2n + d$ coefficients $\tilde{A}_{j,N}$ are required to construct the quadrature rule of order $n$, we actually have to compute $N$ coefficients with $N$ much larger than $n$. The reason is that, the larger the parameter $N$, the smaller the error $R_{j,N}$ for $0 \leq j \leq 2n - 1 + d$.

The foregoing means that when the quadrature formula (4) is calculated using the above method, the accuracy of the results is highly dependent on the size of $N$ (and also on the nature of $G$). All of which brings us to represent the remainder of the modified Gauss formula (4) also depending on $N$.

3. Numerical examples

The choice of $f$ and $G$ is a problem in itself. The design of $G$ is something which experience and common sense must suggest. In order to shed some
light on this matter, each example is accompanied by some hints. Cases in which the effectiveness of this method is visible can be found in the following two sections.

Let $Z(x)$ be a Riemann integrable function on $[a, b]$, $-\infty < a < b < \infty$. Theoretically speaking, the integral of $Z$ can be rewritten as shown below.

$$
\int_a^b Z(x)dx = \frac{(b - a)}{2} \int_{-1}^1 F(x) \frac{dx}{\sqrt{1 - x^2}},
$$

(13)

where $F(x) = Z((b - a)\sqrt{1 - x^2}/2 + (a + b)/2|x|).

As seen in the examples below, other ways of introducing the Chebyshev weight function in the integrand can be used, some of which are simpler than the one given in (13). Also note that the integral on the right side of (13) is ready to be approximated by using the Gauss-Chebyshev rule (2). However, if $F(x)$ is nearly singular then it should produce inaccurate results if the quadrature order is not large enough.

Here we keep the same notation of the previous sections, e.g. $N$ stands for the number of coefficients $A_j$ that are estimated using FFT.

The purpose of this section is to verify the accuracy which is obtained when using the $n$-point (modified) Gauss rule and how it depends on the size of the parameter $N$. It includes comparison with other methods, in particular with the $N$-point Gauss-Chebyshev rule (2).

**Example 3.1.** The following integrals have been studied in [4].

$$
Q_\alpha = \int_{-1}^1 h(x)e^{-\alpha x}dx, \ \alpha > 0.
$$

(14)

The particular case of (14) that we attempt to compute is

$$
Q_{10} = \int_{-1}^1 x^{10}\cos(x)e^{-10x}dx.
$$

(15)

In order to rewrite conveniently the integrand in (15), we put $Q_{10} = I_W(fG)$, where $f(x) = \pi \cos(x)$, $G(x) = \sqrt{1 - x^2}\cosh(-10x)$ and

$$
W(x) = \frac{\sum_{k=0}^{10} \alpha_k T_k(x)}{\pi \sqrt{1 - x^2}},
$$

where $\alpha_{2k+1} = 0$, $k = 0, ..., 4$, and using Matlab we obtain that $\alpha_0 = 0.24609375$, $\alpha_2 = 0.41015625$, $\alpha_4 = 0.234375$, $\alpha_6 = 0.087890625$, $\alpha_8 = 0.01953125$, $\alpha_{10} = 0.001953125$. 

9
Some relative errors produced by \( n \)-point quadrature formula (4) are listed in Table 1. The entries of the last row contains the errors when \( N \)-point Gauss-Chebyshev formula is applied to (15). It is assumed that 621.2996878251843 is the “exact value” of (15).

Table 1: Example 3.1. Errors depending on \( N = 10^s \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( s = 2 )</th>
<th>( s = 3 )</th>
<th>( s = 4 )</th>
<th>( s = 5 )</th>
<th>( s = 6 )</th>
<th>( s = 7 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>7.9e-04</td>
<td>7.2e-06</td>
<td>6.2e-07</td>
<td>7.0e-07</td>
<td>7.0e-07</td>
<td>7.0e-07</td>
</tr>
<tr>
<td>4</td>
<td>7.9e-04</td>
<td>7.9e-06</td>
<td>7.9e-08</td>
<td>7.8e-10</td>
<td>4.1e-12</td>
<td>1.2e-11</td>
</tr>
<tr>
<td>6</td>
<td>7.9e-04</td>
<td>7.9e-06</td>
<td>7.9e-08</td>
<td>7.9e-10</td>
<td>7.9e-12</td>
<td>6.5e-14</td>
</tr>
</tbody>
</table>

\( \text{GC} \)

\( N \) | 7.9e-04 | 7.9e-06 | 7.9e-08 | 7.9e-10 | 7.9e-12 | 8.3e-13 |

Example 3.2. Generalized Fermi-Dirac integrals are defined as

\[
\mathcal{F}(k, \eta, \theta) = \int_{0}^{\infty} \frac{x^k \sqrt{1 + 0.5 \theta x}}{e^{-\eta x} + 1} dx, \quad \eta \in \mathbb{R}, \quad \theta \geq 0.
\]  

(16)

These integrals can be expressed as \( \mathcal{F}(k, \eta, \theta) = \lim_{\delta \to \infty} H_\delta(k, \eta, \theta) \), where

\[
H_\delta(k, \eta, \theta) = \delta^{k+1} \int_{-1}^{1} \frac{|x| \sqrt{1 + 0.5 \theta \delta (1 - x^2)} (1 - x^2)^{k+1/2}}{e^{-\eta \delta (1-x^2)} + 1} dx.
\]  

(17)

The poles of the integrand in (17) coincide with the roots of the equations \( \delta x^2 = (\delta - \eta) - (2k + 1) \pi i, \ k \in \mathbb{Z} \). Just see that when \( \delta \) is large, some of them are close to \([-1, 1]\).

Let \( k = 1/2, \ \eta = -1 \) and \( \theta = 10^{-4} \). If \( \delta = 40 \) then \( H_{40}(1/2, -1, 10^{-4}) \) approximates \( \mathcal{F}(1/2, -1, 10^{-4}) \) up to 15 decimal figures.

Next, we reorganize (17) as \( I_{GW}(f) \) by choosing \( p = (-T_2 + T_0)/2 \),

\[
f(x) = \pi 40^{3/2} \sqrt{1 + 2 \cdot 10^{-3} (1 - x^2)}, \quad G(x) = |x|/(1 + \exp(1 + 40(1 - x^2))).
\]

We have applied the modified Gauss quadrature formula (4) considering the above scheme, and the corresponding errors are displayed in Table 2 (column \( \mathcal{MG} \)). The results in the column marked by the symbol “1/q” are reported in [9] and were obtained by using a Gauss rational rule.
Table 3 attempts to describe the influence of the FFT algorithm in the accuracy of the results. For comparison, the last row lists the errors produced by the $N$-point Gauss-Chebyshev formula. To estimate errors, we have chosen $0.2905124170194927$ as the “exact value” of $H_{10}(1/2, -1, 10^{-4})$ (cf. [8]).

Table 2: Example 3.2. Relative errors when $N = 10^4$. The symbol $\ -- \ $ means that the error is no greater than $5.0e-15$

<table>
<thead>
<tr>
<th>$n$</th>
<th>deg($q$)</th>
<th>$1/q$</th>
<th>$n$</th>
<th>$\mathcal{M}G$</th>
<th>$n$</th>
<th>deg($q$)</th>
<th>$1/q$</th>
<th>$n$</th>
<th>$\mathcal{M}G$</th>
</tr>
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<tbody>
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<td>2</td>
<td>$5.2e-02$</td>
<td>1</td>
<td>$9.6e-04$</td>
<td>4</td>
<td>$8.6e-08$</td>
<td>4</td>
<td>--</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>$1.3e-03$</td>
<td>2</td>
<td>$4.9e-10$</td>
<td>5</td>
<td>$4.0e-07$</td>
<td>5</td>
<td>--</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>$2.7e-05$</td>
<td>3</td>
<td>$4.5e-13$</td>
<td>7</td>
<td>$2.1e-14$</td>
<td>7</td>
<td>--</td>
<td></td>
</tr>
</tbody>
</table>

Table 3: Example 3.2. Errors depending on $N$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$N = 40$</th>
<th>50</th>
<th>75</th>
<th>$10^2$</th>
<th>$10^4$</th>
<th>$10^6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$6.4e-07$</td>
<td>$6.4e-09$</td>
<td>$4.9e-10$</td>
<td>$4.9e-10$</td>
<td>$4.9e-10$</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$6.4e-07$</td>
<td>$5.9e-09$</td>
<td>$4.1e-13$</td>
<td>$4.5e-13$</td>
<td>$4.5e-13$</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$6.4e-07$</td>
<td>$5.9e-09$</td>
<td>$3.6e-14$</td>
<td>--</td>
<td>--</td>
<td></td>
</tr>
</tbody>
</table>

$\mathcal{G}C$

| $N$ | $6.4e-07$ | $5.9e-09$ | $3.2e-14$ | -- | -- | $2.7e-13$ |

**Example 3.3.** Let $\{S(\omega); \omega > 1\}$ be the following class of integrals.

$$S(\omega) = \int_{-1}^{1} \frac{(\pi x/\omega)}{\sin(\pi x/\omega)} dx,$$  \hspace{1cm} (18)

which can be transformed into

$$I_W(F_\omega) = \int_{-1}^{1} \frac{\pi \sqrt{1 - x^2}/\omega}{\sin(\pi \sqrt{1 - x^2}/\omega)} \frac{|x|}{\sqrt{1 - x^2}} dx,$$ \hspace{1cm} (19)
where the integrand $F_\omega(x) = |x|((\pi^2 \sqrt{1 - x^2})/\omega)\sin(\pi \sqrt{1 - x^2}/\omega)$ has singularities near $[-1,1]$ when $\omega \approx 1$. Consequently, we define the polynomials

$$q_n(x) = \prod_{k=1}^n (x^2 - 1 + k^2 \omega^2), \quad n = 1, 2, \ldots.$$  \hspace{1cm} (20)

To apply Eq. (9) we select $f(x) = q_n(x)((\pi^2 \sqrt{1 - x^2})/\omega)\sin(\pi \sqrt{1 - x^2}/\omega)$ and the non-rational factor $G(x) = |x|/q_n(x)$. Column $M\mathcal{G}$ of Table 4 shows the errors when the modified Gauss rule (4) is applied to (19) with $\omega = 1.001$ and $N = 10^5$. The results reported by Gautschi are displayed below the symbol $1/q$ (cf. [9, 11]).

Table 4 allows comparison with Gauss-Chebyshev quadrature formula. The symbol deg$(q)$ stands for the degree of the polynomial (20).

<table>
<thead>
<tr>
<th>$n$</th>
<th>deg$(q)$</th>
<th>$1/q$</th>
<th>$M\mathcal{G}$</th>
<th>$n$</th>
<th>deg$(q)$</th>
<th>$1/q$</th>
<th>$M\mathcal{G}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>4</td>
<td>$8.4e-03$</td>
<td>$8.5e-03$</td>
<td>2</td>
<td>2</td>
<td>$2.9e-02$</td>
<td>$2.9e-02$</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
<td>$1.1e-04$</td>
<td>$1.0e-04$</td>
<td>4</td>
<td>4</td>
<td>$1.9e-05$</td>
<td>$1.2e-05$</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
<td>$9.0e-06$</td>
<td>$8.0e-07$</td>
<td>6</td>
<td>6</td>
<td>$5.0e-06$</td>
<td>$5.4e-09$</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td>$6.2e-06$</td>
<td>$1.0e-08$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5: Example 3.3. Errors depending on $N = 10^s$ ($\text{deg}(q) = 2n$)

<table>
<thead>
<tr>
<th>$n$</th>
<th>$s = 2$</th>
<th>$s = 3$</th>
<th>$s = 4$</th>
<th>$s = 5$</th>
<th>$s = 6$</th>
<th>$s = 7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$1.4e-03$</td>
<td>$8.5e-03$</td>
<td>$8.5e-03$</td>
<td>$8.5e-03$</td>
<td>$8.5e-03$</td>
<td>$8.5e-03$</td>
</tr>
<tr>
<td>4</td>
<td>$7.1e-03$</td>
<td>$6.4e-05$</td>
<td>$1.7e-07$</td>
<td>$8.0e-07$</td>
<td>$8.0e-07$</td>
<td>$8.0e-07$</td>
</tr>
<tr>
<td>8</td>
<td>$7.1e-03$</td>
<td>$6.4e-05$</td>
<td>$6.4e-07$</td>
<td>$6.4e-09$</td>
<td>$6.4e-11$</td>
<td>$6.6e-13$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$G\mathcal{C}$</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$7.1e-03$</td>
<td>$6.4e-05$</td>
</tr>
</tbody>
</table>

Example 3.4. Let $h$ be an integrable function on $[-1,1]$.

$$L(h, \varepsilon, x_0) = \int_{-1}^{1} \frac{h(x)dx}{(x-x_0)^2 + \varepsilon^2}, \quad \varepsilon \neq 0, \quad x_0 \in [-1,1].$$ \hspace{1cm} (21)
These integrals have been considered by Lether [16] and Monegato [17] when $h(x) = e^x$ and $x_0 = 0$. If $\varepsilon$ is small then the integrand may be nearly singular.

Let us write (21) as $I_{W\, G_{\varepsilon,x_0}}$, where $f(x) = \pi h(x)$ and the difficult part is $G_{\varepsilon,x_0}(x) = \sqrt{1 - x^2}((x - x_0)^2 + \varepsilon^2)^{-1}$.

Table 6 displays the effect produced by equations (11) and (12) when these are used to calculate the $n$-point Gauss quadrature formula (4) associated with $G_{\varepsilon,x_0}$. In this case we are evaluating $L(e^x, 10^{-t}, 0.5)$ when $t = 2, 3$ and the respective exact values are assumed to be $5.131681214303589e + 02$ and $5.174840021722350e + 03$. The two rows headed by $N$ list the errors produced by the $N$-point Gauss-Chebyshev rule.

Table 6: Example 3.4 with $h(x) = e^x$. Errors depending on $N = 10^s$

<table>
<thead>
<tr>
<th>$\varepsilon = 10^{-2}$</th>
<th>$n$</th>
<th>$s = 2$</th>
<th>$s = 3$</th>
<th>$s = 4$</th>
<th>$s = 5$</th>
<th>$s = 6$</th>
<th>$s = 7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td></td>
<td>8.8e - 02</td>
<td>6.5e - 09</td>
<td>2.4e - 09</td>
<td>2.5e - 09</td>
<td>2.5e - 09</td>
<td>2.5e - 09</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>8.8e - 02</td>
<td>8.9e - 09</td>
<td>8.8e - 11</td>
<td>8.8e - 13</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\varepsilon = 10^{-3}$</th>
<th>$n$</th>
<th>$s = 2$</th>
<th>$s = 3$</th>
<th>$s = 4$</th>
<th>$s = 5$</th>
<th>$s = 6$</th>
<th>$s = 7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td></td>
<td>5.6e - 01</td>
<td>8.7e - 02</td>
<td>1.5e - 10</td>
<td>2.5e - 10</td>
<td>2.5e - 10</td>
<td>2.5e - 10</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td>5.6e - 01</td>
<td>8.7e - 02</td>
<td>1.0e - 10</td>
<td>8.9e - 14</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>


This section shows how can be applied the modified Gauss rules for evaluating hypersingular integrals when, in addition, the regular part of the integrand is nearly singular. Here we consider Hadamard finite-part integrals which are defined as follows (see [1, 19]).

$$\int_a^b \frac{F(t)dt}{(t-x)^2} = \lim_{\varepsilon \to 0^+} \left( \int_a^{x-\varepsilon} \frac{F(t)dt}{(t-x)^2} + \int_{x+\varepsilon}^b \frac{F(t)dt}{(t-x)^2} - \frac{2F(x)}{\varepsilon} \right), \quad (22)$$

where $a < x < b$. 

13
If the derivative $F'$ satisfies a Lipschitz condition of order $\alpha$ ($0 < \alpha \leq 1$), then the limit in (22) exists.

In this section we tackle the problem of calculating the integral (22) when $F$ is twice differentiable. In practice, the explicit knowledge of the second derivative is not required.

The first step of the procedure is based on the subtraction technique to remove the strong singularity. Let us consider the following equality.

\[
\int_a^b \frac{F(t)dt}{(t-x)^2} = \int_a^b H(x,t)dt + \Phi(x),
\]

where

\[
H(x,t) = \frac{F(t) - F(x) - F'(x)(x-t)}{(t-x)^2}, \quad x \neq t,
\]

\[
H(x,x) = F''(x)/2, \quad \text{and}
\]

\[
\Phi(x) = \frac{F(x)(b-a)}{(a-x)(b-x)} + F'(x) \log \left| \frac{b-x}{a-x} \right|.
\]

We may replace $F'(x)$ by the corresponding centered difference approximation, namely $F'(x) \approx \Delta(x,\eta) = (F(x+\eta) - F(x-\eta))/(2\eta)$, where $\eta > 0$ is chosen moderately small. A drawback is that the results are less reliable.

Preserving the spirit of the above sections, here we also assume that the integration interval is $[-1,1]$. Further we assume that $F(t) = g(t)/w(t)$, where both $g$ and $w$ are smooth, $w(t) > 0$, $t \in (-1,1)$, and $1/w$ can be nearly singular.

From (23) we deduce that $H(x,t) = f(x,t)G(t)/w(x)^2$, where

\[
f(x,t) = \frac{(g(t)w(x) - g(x)w(t))w(x) - w(t)(t-x]\delta(x)}{(t-x)^2},
\]

with $\delta(x) = w(x)g'(x) - w'(x)g(x)$, and $G(t) = 1/w(t)$.

The factor $1/w(x)^2$ can be kept away from the numerical procedure.

A remarkable fact is that $G(t)$ does not depend on $x$, which greatly reduces the computational cost when the integral (22) has to be evaluated for many different values of the parameter.

Since

\[
\int_{-1}^1 \frac{dt}{(t-x)^2\sqrt{1-t^2}} = \int_{-1}^1 \frac{dt}{(t-x)\sqrt{1-t^2}} = 0,
\]

14
then we have that
\[ \int_{-1}^{1} \frac{F(t)dt}{(t-x)^2\sqrt{1-t^2}} = \int_{-1}^{1} \frac{H(x,t)}{\sqrt{1-t^2}}dt, \]
where \(H(x,t)\) is given by Eq. (23).

**Example 4.1.** Set \(g \equiv 1\) and \(w(t) = \sqrt{\alpha^2 - t^2}\) with \(\alpha = 1.1\). Table 7 depicts the errors when \(x = 0.25, N = 2^{12}\) and \(F'(0.25)\) is replaced by the centered difference approximation \(\Delta(0.25, 10^{-7})\). The results in Table 8 are obtained when \(N = 2^{15}\) and the explicit expression of \(F'\) is used in calculations. In both tables, column \(MG\) lists the errors produced by the \(n\)-point Gauss rule, and column “Spline” enumerates the results reported by Palamara [20] when using a method based on splines. In this case the factor \(G(t)\) depends on the parameter \(\alpha\). An explicit expression for this parametric integral can be seen in [19] for every \(|\alpha| > 1\).

<table>
<thead>
<tr>
<th>(n)</th>
<th>(MG)</th>
<th>Spline</th>
<th>(n)</th>
<th>(MG)</th>
<th>Spline</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.7e-02</td>
<td></td>
<td>16</td>
<td>6.6e-08</td>
<td>3.8e-03</td>
</tr>
<tr>
<td>4</td>
<td>1.8e-03</td>
<td></td>
<td>32</td>
<td>7.0e-08</td>
<td>4.5e-04</td>
</tr>
<tr>
<td>8</td>
<td>1.9e-05</td>
<td>7.9e-02</td>
<td>64</td>
<td>7.2e-08</td>
<td>2.7e-05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>(n)</th>
<th>(MG)</th>
<th>Spline</th>
<th>(n)</th>
<th>(MG)</th>
<th>Spline</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.7e-02</td>
<td></td>
<td>16</td>
<td>4.6e-09</td>
<td>3.8e-03</td>
</tr>
<tr>
<td>4</td>
<td>1.8e-03</td>
<td></td>
<td>32</td>
<td>1.1e-09</td>
<td>4.5e-04</td>
</tr>
<tr>
<td>8</td>
<td>1.9e-05</td>
<td>7.9e-02</td>
<td>64</td>
<td>1.1e-09</td>
<td>2.7e-05</td>
</tr>
</tbody>
</table>

5. **Notes on computational cost**

The examples in Section 3 suggest that the following empirical relation
\[ \mathcal{E}_{n,N}^M(f) \approx \mathcal{E}_{N}^{G}\mathcal{G}(fG), \quad n \ll N, \]
should be true in general. That is, the relation between accuracy and the number of functional evaluations that actually are carried out is practically the same for both methods, the modified Gauss rule and the Gauss-Chebyshev quadrature formula. Nevertheless, the main purpose of this section is to report on some experimental results which allow to conclude that in some cases the proposed method is less costly than the classical quadrature formula. For this we consider again (21) with \( f_p(x) = \pi \prod_{k=1}^{p} \log(x^2/k + e) \), \( x_0 = 0 \) and \( \varepsilon = 10^{-3} \).

Firstly, it is intended to compare the execution time consumed by each of the two procedures, the 8-point Gauss rule (\( MG \)) associated with the difficult factor \( G(x) = \sqrt{1 - x^2/(x^2 + \varepsilon^2)} \) and the \( N \)-point Gauss-Chebyshev rule (\( GC \)). Secondly, they are mentioned two cases in which modified Gauss rules are particularly effective.

Table 9 shows the time of computation \( t_{r,s} \) for both procedures when \( p = 10^r \), \( r = 0, 3 \); and \( N = 10^s \), \( s = 2, \ldots, 7 \). From these results we can see that when running the Gauss Chebyshev rule, timings depend sensitively on the complexity of the function \( f_p \), which is a very predictable result. The numbers in Table 9 are average values obtained using a CPU with a clock rate of 2.27 GHz.

<table>
<thead>
<tr>
<th></th>
<th>( r )</th>
<th>( s = 2 )</th>
<th>( s = 3 )</th>
<th>( s = 4 )</th>
<th>( s = 5 )</th>
<th>( s = 6 )</th>
<th>( s = 7 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( MG )</td>
<td>0</td>
<td>2.0e-04</td>
<td>5.1e-04</td>
<td>2.5e-03</td>
<td>2.6e-02</td>
<td>3.0e-01</td>
<td>3.9e+00</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>2.1e-03</td>
<td>2.7e-03</td>
<td>4.5e-03</td>
<td>2.9e-02</td>
<td>3.1e-01</td>
<td>3.9e+00</td>
</tr>
</tbody>
</table>

| \( t_{3,s}/t_{0,s} \) | 1.0e+01 | 5.3e+00 | 1.8e+00 | 1.1e+00 | 1.0e+00 | 1.0e+00 |

| \( GC \) | 0   | 1.3e-04 | 5.3e-04 | 1.9e-03 | 1.1e-02 | 1.1e-01 | 1.1e+00 |
|       | 3   | 7.7e-03 | 6.4e-02 | 6.3e-01 | 3.7e+00 | 3.9e+01 | 3.9e+02 |

| \( t_{3,s}/t_{0,s} \) | 5.9e+01 | 1.2e+02 | 3.3e+02 | 3.4e+02 | 3.5e+02 | 3.5e+02 |

Basically, the procedure we use to compute the modified Gauss rule consists of two well-known algorithms, namely the \( FFT \) and the modified Chebyshev algorithm. The complexity of the former is \( \mathcal{O}(N \log(N)) \), while the latter requires \( \mathcal{O}(n^2) \) arithmetic operations, which is practically negligible compared to the cost caused by the \( N \) functional evaluations that precedes the application of the \( FFT \).
Prior results do not only show some overlap between the modified Gauss formula and Gauss-Chebyshev formula, but also some differences. As known, the classical integration rule performs $N$ functional evaluations of the whole integrand $F = fG$. Instead, after decomposing the integrand into two factors, the modified Gauss rule evaluates the function $G$ at $N$ points, and besides it only evaluates $f$ at $n$ points, where $n \ll N$. Hence, in some cases the modified Gauss formula can be less costly than the Gauss-Chebyshev formula. This may occur when the complexity of $f$ is high, as can be seen in Table 9, or when $G$ is fixed and $I_{GW}(f)$ has to be computed for many different functions $f$ (Section 4). This latter case can also be illustrated by considering the problem of evaluating the Laplace transform of a non standard function $F(t)$, for several values of the parameter.

By changing the variables conveniently, we obtain

$$
\int_0^\infty e^{-st}F(t)dt \approx \int_{-1}^1 \frac{f_{\delta,s}(t)G_{\delta}(t)}{\sqrt{1-t^2}} dt,
$$

where $f_{\delta,s}(t) = (\delta/2s)F(\delta(t+1)/2s)$, $G_{\delta}(t) = \sqrt{1-t^2} \exp(-\delta(t+1)/2)$ and $\delta > 0$ is suitably chosen.

Note that $G_{\delta}$ does not depend on $s$. Moreover, the above analysis includes technical aspects that have already been treated in Section 3.

6. Concluding remarks

It is proposed a simple method to calculate the weights and nodes of the so-called modified Gauss rule, specially when the modifying factor is nearly singular. Thereby, we can evaluate with high accuracy some definite integrals whose mass is distributed unevenly. One of the key elements of this approach is the relationship between modified moments and the coefficients of the Chebyshev series expansion of the difficult part of the integrand.

The numerical results which have been obtained using modified Gauss rules appear to be fairly good when compared with those produced by a very effective quadrature formula of rational type. Regarding computational cost, experimental results indicate that when considering integrals like the ones in Section 4 and 5, our method should run faster than the Gauss-Chebyshev rule. This is because the latter has to absorb the complexity of the integrand in its entirety. However, Section 3 shows that the accuracy is not better than that of the Gauss-Chebyshev rule when the comparison is made according to the number of functional evaluations.
Finally, we conclude that this approach can be seen as a valid alternative when it comes to evaluating the integral of a difficult function. However, one drawback to bear in mind is that the proposed approach depends heavily on expert judgment. In this regard, it is hoped that the examples in this document will help to improve the reader’s experience.

Acknowledgments

The authors thank the referees for helpful remarks and suggestions.

References


