Evaluation of finite part integrals using a regularization technique that decreases instability

J. Illán-González\textsuperscript{a,*}, J.M. Rebollido-Lorenzo\textsuperscript{b}

\textsuperscript{a}Universidad de Vigo, PO-36310, Pontevedra, Spain
\textsuperscript{b}High school of Valga, PO-36645, Xunta de Galicia, Pontevedra, Spain.

Abstract

A hypersingular integral can be regularized by replacing the whole integrand by a forward difference quotient of 2nd order. If the density function is nearly singular, then Gauss quadrature formulas associated with a suitable modification of the Chebyshev weight function allow to obtain great precision with few nodes. However, in most cases, the own nature of this procedure makes unpredictable the location of quadrature nodes. This paper presents a simple but effective technique whose aim is to mitigate instability when some node lies too close to the pole. Some numerical examples are shown to evaluate the performance of the proposed method.

Keywords: Hyper-singular integral, Gauss quadrature formula, Chebyshev series method, nearly singular function.

2000 MSC: 41A55, 65D32, 41A21

1. Introduction

A hypersingular integral over the interval \((-1, 1)\) is defined as the following limit (if exists).

\[
\int_{-1}^{1} \frac{F(t)dt}{(t-x)^2} = \lim_{\varepsilon \to 0} \left( \int_{-1}^{x-\varepsilon} \frac{F(t)dt}{(t-x)^2} + \int_{x+\varepsilon}^{1} \frac{F(t)dt}{(t-x)^2} - \frac{2F(x)}{\varepsilon} \right), \quad (1)
\]

where \(x \in (-1, 1)\) is the Hadamard-type singularity of order two.

To ensure the existence of \((1)\), it suffices that \(F'' \in \text{Lip}_\alpha\), \(0 < \alpha \leq 1\), although this assumption can be weakened \[2\].

\*Corresponding author
The calculation of singular boundary integrals is a problem that arises from the application of the boundary element method (BEM), and is related to the evaluation of (1). Indeed, a non-trivial discretization process must be carried out to transform a boundary integral, defined on a two-dimensional region, into one of type (1) (cf. [2, 3]). On the role played by these integrals in elasticity, mechanics, etc, we refer the reader to [4, 5], and references therein.

The following approximation formula is equivalent to (1) (cf. [6]).

\[
\int_{-1}^{1} \frac{F(t)dt}{(t-x)^2} = \lim_{\varepsilon \to 0^+} \left( \int_{-1}^{1} \frac{(t-x)^2 F(t)dt}{((t-x)^2 + \varepsilon^2)^2} - \frac{\pi F(x)}{2\varepsilon} \right) - \frac{F(x)}{1-x^2},
\]

(2)

Note that both (1) and (2) are approximation formulas depending on a parameter \(\varepsilon\). They have a theoretical value but are not appropriate for numerical calculation. One fact is that a great variety of methods to evaluate integrals with strong singularities are currently known, most of which have been published after the sixth decade of the 20th century (cf. [5, 7, 8]).

When \(\varepsilon\) is small, the integrals on the right side of (2) are nearly hypersingular, an issue also treated by several authors due to the important role they play in the applications of the BEM (cf. [9, 10]).

Our approach is mainly based on replacing the integrand of the integral defined in (1) by the following forward difference quotient.

\[
E(x, t) = \frac{F(t) - F(x) - F'(x)(t-x)}{(t-x)^2}.
\]

(3)

Paget [11] seems to be one of the first in using (3) to remove the singularity of (1). Nevertheless, when using finite precision arithmetic and \(x \approx t\), then \(E(x, t)\) is unstable, even when \(F''(x)\) exists.

Other than (3), there are diverse regularization techniques that can be applied to (1). Following the same approach as that indicated by (3), if the order of the Hadamard-type singularity is \(m > 2\), then one may use the Taylor polynomial of \(F(t)\) with degree \(m - 1\), and centered at \(t = x\) (cf. [12]). However, a more effective variant seems to be the use of the polynomial \(P(\rho)\) that interpolates the non-singular part of the integral at a uniform mesh of points, and \(\rho\) is the distance between the singularity and the integration variable (cf. [2, 3]). According to the results reported in [2, 3], a maximum accuracy of 8 decimal digits can be achieved when using a sixth-order Gauss quadrature formula.
Regardless of the robustness shown by the method used in [2], the quality of the results should be further enhanced using the barycentric formulation based on $n$-point sets with an asymptotic density proportional to the Chebyshev weight function of the first kind as $n \to \infty$. A well known fact is that polynomial interpolation based on equidistant points is ill-conditioned [13].

All the above mentioned methods assume that $F(t)$ is regular, and focus on removing the polar singularity. Instead, we are interested in evaluating (1) when $F$ behaves poorly, a problem whose solution is connected with the numerical stability of (3). Then, our starting point is to assume that $F(t) = g(t)H(t)$, where $H$ represents the component of $F$ that is related to numerical instability. In short, $H$ is nearly-singular and $g$ is smooth.

In a previous paper [14] we used Gauss quadrature formulas associated with a suitable modification of the Chebyshev weight function to evaluate the integral of the parametric function (3). The calculation of the corresponding quadrature weights and nodes relies on the existing relation between the modified moments and the coefficients of the Chebyshev series expansion of $H(t)\sqrt{1-t^2}$. As a result, the nodes are not known in advance, since they depend on the function $H(t)$ we have selected. The only information available a priori is that the asymptotical distribution of nodes is $1/(\pi \sqrt{1-t^2})$ [15]. This may cause that some node is located very close to the parameter $x$, with the consequent loss of digits (cf. [5, 16, 17]).

In line with previous comments, the purpose of this work is to show how the forward difference quotient (3) can be integrated efficiently regardless of the location of quadrature nodes and singular points. For this we propose a new type of regularization of the integral (1) which consists in conveniently introducing an additional parameter within (3). All of which is organized in the paper as follows.

As for the problem of calculating the parameters of the quadrature formula, we describe in Section 2 a fairly general method that improves the results obtained in [14]. This section also addresses some aspects of Gauss quadrature formulas associated with a weight function partially modified by a rational function, a topic suggested by W. Gautschi in 2004. In Section 3 we describe the $\varepsilon$-regularization that we apply when the distance between nodal and collocation points is very small. Some examples are given in Section 4 to show the performance of our method. Finally, Section 5 contains some remarks as conclusion.
2. Preliminaries

Let us put $W_\pi(t) = W(t)/\pi$, where $W(t) = 1/\sqrt{1 - t^2}$.

Let $f$ be a real function defined on $[-1, 1]$. If $f$ is bounded, then the uniform norm of $f$ is $\|f\| = \sup\{|f(t)|; t \in [-1, 1]\}$.

Let $f$ be a real function defined on $[-1, 1]$. If $f$ is bounded, then the uniform norm of $f$ is $\|f\| = \sup\{|f(t)|; t \in [-1, 1]\}$.

Let $\|f\|_{p,W} = \left(\int_{-1}^{1} |f(x)|^p W(x) dx\right)^{1/p}$, where $p \geq 1$. Let $L_{p,W}$ denote the vector space of measurable functions $f$ such that $\|f\|_{p,W} < \infty$.

The symbol $T_n$ stands for the $n$th orthogonal polynomial associated with $W$, defined as $T_n(x) = \cos(n\theta)$, where $x = \cos(\theta)$.

2.1. Notes on Chebyshev series

Let $\sum_{j=0}^{\infty} c_j T_j(x)$ be the Chebyshev series expansion of $f \in L_{2,W}$, where the prime indicates that the first term in the sum is halved. Moreover, the coefficients $c_j$ are given by (cf. [18, section 5.2])

$$c_j = 2 \int_{-1}^{1} T_j(t) f(t) W_\pi(t) dt.$$ \hspace{1cm} (4)

The following lemma collects three different results which link the speed of convergence of $S_n(f)$ (the $n$th partial sum of the Chebyshev series expansion of $f$) with the smoothness of $f$ (cf. [18, Theorems 5.2, 5.14, 5.16]).

**Lemma 2.1.**

1. If $f \in L_{2,W}$, then $\lim_n \|f - S_n(f)\|_{2,W} = 0$.

2. If the $(m+1)$st derivative $f^{(m+1)}$ exists, and also is continuous, then $\|f - S_n(f)\| = O(n^{-m})$.

3. Let $\Gamma_\rho := \{z : |z - \sqrt{z^2 - 1}| = \rho\}$, with $0 < \rho < 1$. Suppose that $f$ is analytic on the interior of $\Gamma_\rho$. Then $\|f - S_n(f)\| = O(\rho^n)$.

The information required about the convergence rate of $S_n(f)$ can be obtained by studying the asymptotic behavior of $[4]$, as $j \to \infty$. Examples of slowly convergent series are the ones corresponding to $f(t) = \sqrt{1 - t^2}$ and $f(t) = |t|$, $|t| \leq 1$, whose coefficients have been calculated explicitly (cf. [18]).

The Chebyshev series of $f(t) = H(t) \sqrt{1 - t^2}$ could converge slowly, even when $H$ is infinitely differentiable (cf. [19]). In fact, if $c_n$ is the $n$th Chebyshev coefficient of $f(t)$, then $H(\pm 1) = 0$ is one of the conditions to be assumed to obtain that $c_n = O(n^{-p})$, $p > 2$. If $H \equiv 1$, then $c_n \approx 1/n^2$ ($n \to \infty$). On the other hand, when $q$ is a polynomial whose zeros are located outside the interval $[-1, 1]$, the Chebyshev series of $1/q$ converges geometrically with a speed that depends on the distance between the interval $[-1, 1]$ and the zeros of $q$ (Lemma 2.1).
2.2. A quadrature formula w.r.t. a modified Chebyshev weight

Suppose that $G, H \in L^2_W$ are non-negative on $[-1, 1]$. We want to evaluate the integral $\int_{-1}^{1} F(t)W_\pi(t)dt$, where $F(t) = f(t)G(t)H(t)$, and $f(t)$ is smooth. For this, we will consider the following quadrature formula associated with $G(t)H(t)W_\pi(t)$. It is defined as follows.

$$\int_{-1}^{1} f(t)G(t)H(t)W_\pi(t)dt = \sum_{j=1}^{n} \lambda_{n,j} f(x_{n,j}) + \mathcal{E}_n(f), \quad (5)$$

where $\mathcal{E}_n(f)$ is the quadrature error, the weights are given by

$$\lambda_{n,j} = \int_{-1}^{1} \frac{Q_n(t)}{Q_n(x_{n,j})(t-x_{n,j})}G(t)H(t)W_\pi(t)dt, \quad j = 1, \cdots, n, \quad (6)$$

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

The quadrature defined by (5)–(6) possesses maximum degree of exactness, so that all hitherto known results related to convergence of Gaussian quadrature rules can be applied to it. What could be an interesting issue is to establish convergence not only in terms of the smoothness of the integrand $f$, but also in terms of the nature of both functions $G$ and $H$, a problem that is beyond the scope of this article. However, we refer the reader to [20] whose technique can also be applied to formula (5) when $H$ is replaced by a sequence of the type $H_n = 1/q_n$, where $q_n$ stands for a polynomial with $\text{deg}(q_n) \in \Gamma \subset \mathbb{N}$. So it is studying (5) by using the connection with multipoint Padé approximation to Markov functions of the form $\int_{-1}^{1} G_m(t)(t-z)^{-1}W(t)dt$, where $z \in \mathbb{C} \setminus [-1,1]$ and $\{G_m\}$ is a polynomial sequence such that $\|G_m - G\|_{1,W} \to 0$, as $m \to \infty$.

Under the above assumptions, the two equations (5) and (6) define a quadrature formula of rational type for each $m$, and the corresponding analysis of the global error $\mathcal{E}_{n,m}(f)$ can be done as follows.

$$|\mathcal{E}_{n,m}(f)| \leq |\mathcal{R}_{m}^{(a)}(f)| + |\mathcal{R}_{n,m}^{(b)}(f)|,$$

where $\mathcal{R}_{m}^{(a)}(f) = \int_{-1}^{1} f(x)(G(x) - G_m(x))W(x)dx$, and

$$\mathcal{R}_{n,m}^{(b)}(f) = \int_{-1}^{1} f(x)G_m(x)W(x)dx - \sum_{j=1}^{n} \lambda_{n,m,j} f(x_{n,m,j}), \quad (7)$$
and the weights are now defined as
\[ \lambda_{n,m,j} = \int_{-1}^{1} \frac{q_n(x_{n,m,j}) Q_{n,m}(t)}{Q'_{n,m}(x_{n,m,j})(t-x_{n,m,j})} \frac{G_m(t)}{q_n(t)} W_\pi(t) dt, \quad j = 1, \ldots, n, \]
where \( Q_{n,m} \) is the \( n \)th orthogonal polynomial associated with \( G_m W_\pi / q_n(t) \), and the nodes \( x_{n,m,j} \) are the zeros of \( Q_{n,m} \).

It is clear that \( R_n^{(a)}(f) \to 0 \), as \( m \to \infty \), for every \( f \in L_\infty W \). Furthermore, \( R_n^{(b)}(p/q_n) = 0 \), \( p \in \Pi_{2n-1} \), \( m \in \mathbb{N} \).

A slight modification of the proof of [20, Proposition 4] allows to estimate (7). It can be done when \( f \) is analytic on \([-1,1]\), also meromorphic in a neighborhood \( V \) of \([-1,1]\), and there exists \( n_0 \) such that \( q_n f \) is analytic on \( V \) when \( n > n_0 \). In a sense, the resulting estimate depends on \( V \), and can also be expressed in terms of the asymptotic behavior of \( \deg(q_n) \) as \( n \to \infty \), by assuming that \( \liminf_n \deg(q_n)(2n)^{-1} = \sigma, \ 0 < \sigma \leq 1 \). Then, it is possible to find \( \delta \in (0,1) \), such that
\[ \limsup_n \left| R_n^{(b)}(f) \right|^{1/(2n)} \leq \delta^\sigma. \]
The degree of \( q_n \) is usually chosen according to the number of poles that are really affecting the scale of the integrand. The two cases \( n = \deg(q_n) \) (\( \sigma = 1/2 \)) and \( 2n = \deg(q_n) \) (\( \sigma = 1 \)) are considered in most published papers dealing with this topic. The aim of this dichotomy is to check the role played by \( \deg(q_n) \) in the numerical process.

Next, we tackle the problem of calculating weights and nodes of the quadrature defined by (5)–(6).

2.3. Calculation method
As for singular integrals, it may happen that the misbehavior of the integrand not only occurs by the presence of difficult poles. In such situation, the option of using a rational factor to remove singularities may be not the best. Despite the examples worked by Van Assche [21], in those cases in which the integrand behaves exponentially, the standard rational approach for numerical quadrature does not indicate clearly what should be the design of the rational function that must be used to transform the integrand into another smoother. Presumably motivated by this shortcoming Gautschi [22, Remark to Theorem 3.25] suggested a modification of the form \( G/q \), where \( G \) is not related to the poles of the integrand but is partially associated with
instability, and \( q \) is a polynomial whose zeros are equal to some poles of the integrand. Unfortunately, Gautschi did not elaborate on it. A viable approach might be the one given by \([5] [6]\), choosing \( H = 1/q \).

In the following a numerical procedure that is derived from \([14]\) is described. Besides, it covers the numerical implementation of the quasi-rational formulas suggested by Gautschi. For this, we replace the initial formulation of the problem by a convenient modification of the Chebyshev weight function of the first kind to which applies the modified moments algorithm. According to the previous subsection, the modification factor we propose is \( GH \), where both \( G \) and \( H \) are approximated by real-valued polynomials with the aim of computing modified moments.

Here we will apply a well known method that has been used for estimating nodes and weights of any Gauss formula. This procedure depends on the knowledge of the coefficients \( \{a_k, b_k\} \) of the following recurrence relation satisfied by the nodal polynomials appearing in Eq. (6).

\[
Q_{k+1}(t) = (x - a_k)Q_k(t) - b_kQ_{k-1}(t),
\]

with \( Q_0 \equiv 1 \), \( Q_{-1} \equiv 0 \), and \( b_k > 0 \), \( k = 0, 1, \ldots \). Unfortunately, both the coefficients and polynomials are unknown, and to top they all depend on how we choose \( G \) and \( H \).

For solving this problem we use the modified moments algorithm. In this specific case, it is expected that this procedure is well conditioned when the moments are given in terms of the Chebyshev orthogonal polynomials of the first kind (See Section \([2]\)). The detailed description of this procedure can be found in \([22] [24]\). Here we only discuss the problem of calculating the so-called modified moments given in terms of the following integrals

\[
\mu_{m,0} = \int_{-1}^{1} P_m(t)G(t)H(t)W_\pi(t)dt, \ m = 0, 1, \ldots, 2n - 1, \quad (8)
\]

where \( P_m \) is the \( m \)th monic Chebyshev polynomial of the first kind.

A crucial step is the calculation of the first \( N \) coefficients of the Chebyshev series expansions of \( G \) and \( H \):

\[
G(t) \sim \sum_{j=0}^{\infty} A_j T_j(t), \quad H(t) \sim \sum_{k=0}^{\infty} B_k T_k(t), \quad (9)
\]

where the coefficients \( \{A_j\} \) and \( \{B_k\} \) are given by \([4]\).
The following approximation formula establishes a link between (8) and (9) (cf. [14]).

\[ \mu_{m,0} \approx S_M = D_m \sum_{k=0}^{M} B_k (A_{|k-m|} + A_{k+m}), \quad m = 0, \ldots, 2n - 1. \]  

(10)

where \( \mu_{m,0} = \lim_{M \to \infty} S_M \), \( D_m = 2^{-(m+1)} \), if \( m \geq 1 \), and \( D_0 = 2^{-2} \). The two primes on the summation symbol indicate that both \( A_0 \) and \( B_0 \) are halved.

What usually happens is that the parameter \( M \) in (10) is much smaller than \( N \), where \( N \) is the number of Chebyshev coefficients that has been calculated.

It may be that at least one of the sequences \( \{A_n\} \) and \( \{B_n\} \) is known explicitly, which implies a simplification of the calculations and an increasing of the accuracy. In any event, the Chebyshev coefficients of \( G \) and \( H \) can always be estimated by using Chebyshev interpolation [18] or FFT.

The sequence \( \{B_k (A_{|k-m|} + A_{k+m})\} \) should converge to zero much faster than the sequence of Chebyshev coefficients of the product \( GH \). As shown in [14], if \( H \) is a polynomial of degree \( d \), then the series in Eq. (10) is a finite sum with \( d + 1 \) terms. If \( H \equiv 1 \), then the modified moments are calculated using the following relation

\[ \mu_{m,0} = A_m / 2^m, \quad m = 1, \ldots, 2n - 1, \quad \mu_{0,0} = A_0 / 2. \]  

(11)

In some cases, the simplicity of (11) has as its counterpart that \( \{A_k\} \) may converge slowly to zero, which would involve a lot of calculations.

The complexity of the modified moments algorithm is \( O(n^2) \). Besides, it is well known that FFT is of order \( O(N \log(N)) \) and that, the larger the \( N \), the more accurate the calculation of the first coefficients. In order to facilitate the application of the Matlab function \texttt{fft}, we have used the formulas given in [14, 25] for this purpose. As [14], here it holds that \( n \ll N \).

3. \( \epsilon \)-regularization

Let \( E(x, t) \) be as in (3). When using floating-point arithmetic the calculation of \( F''(x) \) by means of \( E(x, x + \delta) \) must be carried out by choosing \( \delta \) adequately, e.g., \( \delta = (24u ||F|| / ||F''||)^{1/3} \), where \( u \) denotes the unit roundoff. If \( \delta = t - x \) then the issue may worsen when \( x \) is given in advance and the
value of \( t \) is unpredictable. To overcome this drawback we have introduced an additional parameter in \( E(x,t) \) as shown below.

\[
E(x,t,\varepsilon) = \frac{F(t(1-\varepsilon)) - F(x) - F'(x)(t(1-\varepsilon) - x)}{(t(1-\varepsilon) - x)^2},
\] (12)

where \(-1 < x < 1, 0 \leq \varepsilon < 1\).

Taking into account (12) and previous comments, now it follows that \( \delta = (t(1-\varepsilon) - x) \). Therefore, there must be a simple relationship between \( \varepsilon \) and \( \delta \) when \( |t - x| \) is too small. In fact, according to our purposes the variable \( t \) must range over a set \( \{x_{n,k}\}_{k=1}^n \) formed by the nodes of the \( n \)th quadrature (5). Suppose further that for some \( k, x_{n,k} \neq 0 \), and the number \( |x_{n,k} - x| \) is almost negligible related to the accuracy of the machine, then \( \varepsilon \) and \( \delta \) satisfy \( |x_{n,k}| \approx |\delta| \).

Notice that \( E(x,t) = E(x,t,0) \). Moreover, if \( F(x) \) is 3 times differentiable at the point \( x, x \neq 0 \), then

\[
\lim_{\varepsilon \to 0} E(x,x,\varepsilon) = \frac{F''(x)}{2}.
\] (13)

Eq. (13) is obtained from Taylor’s theorem: \( E(x,x,\varepsilon) = F''(x)/2 + \xi(\varepsilon) \), where \( \xi(\varepsilon) \) is a function such that \( \lim_{\varepsilon \to 0} \xi(\varepsilon) = 0 \).

Because \( E(0,0,\varepsilon) = 0/0 \), the point \( x = 0 \) is considered as a singularity of (12). This indetermination is attenuated if, following (2), we replace the denominator of \( E(x,t,\varepsilon) \) by \( (t(1-\varepsilon) - x)^2 + \tau(\varepsilon) \), where \( \tau \) is non-negative and \( \tau(\varepsilon) = o(\varepsilon^2) \), so that \( E(0,0,\varepsilon) = 0 \). Unfortunately, in most cases \( F''(0) \neq 0 \). Furthermore, the presence of \( \tau(\varepsilon) \) makes the theory a bit more complicated and brings little in the experimental practice. Instead, the following modification of (12) has shown to be more adequate when calculations are performed using a finite precision arithmetic.

\[
E_u(x,t,\varepsilon) = \frac{F(t(1-\varepsilon)) - F(x) - F'(x)(t(1-\varepsilon) - x)}{(t(1-\varepsilon) - x)^2 + u}, \quad 0 \leq \varepsilon < 1.
\] (14)

Thus, for \( \varepsilon \) suitably small, it follows that

\[
\int_{-1}^{1} \frac{F(t)dt}{(t-x)^2} \approx \int_{-1}^{1} E_u(x,t,\varepsilon)dt - \frac{2F(x)}{1-x^2} + F'(x) \log \left( \frac{1-x}{1+x} \right).
\] (15)
Lemma 3.1. Let \( w \) be a weight function such that \( |t - x|^\alpha - 1 \in L_{1,w}, \alpha \in (0,1), x \in (-1,1) \). If \( F' \in \text{Lip}_\alpha \), then for all \( \varepsilon \in (0,1) \), it holds that
\[
\int_{-1}^{1} |E(x,t,\varepsilon)|w(t(1-\varepsilon))dt \leq \frac{K_\alpha}{1-\varepsilon} \int_{-1}^{1} \frac{w(t)dt}{|t-x|^{1-\alpha}},
\]
(16)
where \( K_\alpha > 0 \) is a Lipschitz constant for \( F' \).

Notice that the upper bound in (16) depends essentially on \( x \). The proof of Lemma 3.1 is performed by putting \( u = t(1-\varepsilon) \) and applying the mean value theorem.

The following two propositions cover both pointwise and uniform convergence as \( \varepsilon \to 0 \), with respect to the parameter \( x \in (-1,1) \).

Proposition 3.1. Let \( R(x,\varepsilon) \) be defined as
\[
R(x,\varepsilon) = \int_{-1}^{1} E(x,t,\varepsilon)dt - \int_{-1}^{1} E(x,t)dt, \quad 0 < \varepsilon < 1, \ |x| < 1.
\]
If \( F' \in \text{Lip}_\alpha, \ 0 < \alpha \leq 1 \), then the following assertions hold true.

I. \( |R(x,\varepsilon)| \leq K\varepsilon \), where \( \varepsilon \) is small and \( K > 0 \) depends on both \( x \) and \( F \).

II. \( \sup_{|x|<1} |R(x,\varepsilon)| = O(\varepsilon^\alpha), \ (\varepsilon \to 0) \).

Proof. As in Lemma 3.1, we replace \( t \) by \( t(1-\varepsilon) \) to obtain
\[
R(x,\varepsilon) = \int_{-1}^{1-\varepsilon} \frac{\varepsilon E(x,t)}{1-\varepsilon} dt - \int_{-1}^{1-\varepsilon} E(x,t)dt - \int_{1-\varepsilon}^{1} E(x,t)dt.
\]
As regards to assertion I, let us assume that \( x \) is fixed and \( \varepsilon \) satisfies \( |x| < 1 - \varepsilon \). Let \( \delta \in (0,1) \) and also suppose that \( 0 < \varepsilon < \delta \). From the assumptions above we obtain that
\[
\left| \int_{-1}^{1-\varepsilon} \frac{\varepsilon E(x,t)}{1-\varepsilon} \right| \leq \frac{K_\alpha \varepsilon}{1-\varepsilon} \int_{-1}^{1} \frac{dt}{|t-x|^{1-\alpha}} \leq \frac{2K_\alpha \varepsilon}{\alpha(1-\delta)}, \ 0 < \alpha \leq 1.
\]
On the other hand, if \( |x| < 1 - \delta \), then
\[
\int_{-1}^{1-\varepsilon} |E(x,t)|dt \leq K_\alpha \int_{-1}^{1-\varepsilon} \frac{dt}{|t-x|^{1-\alpha}} \leq \frac{\varepsilon K_\alpha}{(x+1-\delta)^{1-\alpha}}.
\]
To prove II we note that \(|\int_{-1+\varepsilon}^{1-\varepsilon} E(x,t)dt|\) is bounded as \(\varepsilon \to 0\), even when \(x\) varies freely outside the interval \([-1+\varepsilon, 1-\varepsilon]\).

Now suppose that \(-1 < x \leq -1+\varepsilon\). Then
\[
\int_{-1}^{-(1-\varepsilon)} |E(x,t)|dt \leq \int_{-1}^{-(1-\varepsilon)} \frac{K_\alpha dt}{|t-x|^{1-\alpha}} = \frac{K_\alpha}{\alpha} \left( (x+1)^\alpha + (-1+\varepsilon-x)^\alpha \right) \leq \frac{2^{1-\alpha} K_\alpha \varepsilon^\alpha}{\alpha}.
\]
If \(-1+\varepsilon < x\), then \(x-t \geq -1+\varepsilon-t\) for all \(t \in [-1,-1+\varepsilon]\). Hence
\[
\int_{-1}^{-(1-\varepsilon)} |E(x,t)|dt \leq K_\alpha \int_{-1}^{-(1-\varepsilon)} \frac{dt}{(-1+\varepsilon-t)^{1-\alpha}} \leq \frac{\varepsilon^\alpha K_\alpha}{\alpha}.
\]

The previous upper bounds when the integral is over \([-1,-1+\varepsilon]\) also hold when it is over \([1-\varepsilon, 1]\), so the proof finishes. \(\square\)

**Proposition 3.2.** If \(F' \in \text{Lip}_\alpha\), \(0 < \alpha \leq 1\), and \(|x| < 1\), then it holds that
\[
\int_{-1}^{1} \frac{E(x,t,\varepsilon)}{\sqrt{1-t^2(1-\varepsilon)^2}} dt - \int_{-1}^{1} \frac{E(x,t)}{\sqrt{1-t^2}} dt = O(\varepsilon^{1/2}), \ (\varepsilon \to 0).
\]

**Proof.** Let \(\delta \in (0,1)\) be fixed and such that \(|x| < 1-\delta\). Let \(0 < \varepsilon < \delta < 1\). The proof is based on Lemma [3.1] and
\[
\int_{-1}^{1+\varepsilon} \frac{dt}{|t-x|^{1-\alpha}\sqrt{1-t^2}} \leq \frac{\pi - \arccos(-1+\varepsilon)}{(x+1-\varepsilon)^{1-\alpha}} \leq \frac{K\varepsilon^{1/2}}{(x+1-\delta)^{1-\alpha}},
\]
where \(K > 0\) is an absolute constant. \(\square\)

Proposition [3.2] can be easily extended to any weight function \(w(t)\) such that \(\int_{-1+\varepsilon}^{1+\varepsilon} w(t)dt = O(\varepsilon^\beta), \ (\varepsilon \to 0)\), for some \(\beta \in (0,1]\).

### 4. Numerical tests

In all the examples given below, the first \(N\) coefficients of the Chebyshev series expansion of a given function are estimated using \(FFT\), unless an explicit formula is known. When neither of the two factors \(G\) and \(H\) is a constant function, the modified moments are estimated using (10). If one of them is constant, then Eq. (11) is applied.
4.1. A quasi–rational modification

The example below shows that a non–rational modification can yield an accuracy superior to that obtained by rational quadratures, although in some cases the overall complexity is similar to that obtained using the classical Gauss–Chebyshev rule (cf. [14]).

Example 4.1. $S(\omega) = \int_{-1}^{1} \frac{\pi t/\omega}{\sin(\pi t/\omega)} dt, \omega > 1$ (cf. [14, 22, 26]).

When $\omega$ is close to 1, we may multiply the integrand by the polynomial

$$q_n(x) = \prod_{k=1}^{n} (k^2 \omega^2 - x^2),$$

where $n$ is chosen according to the number of poles that must be neutralized. In order not to modify the integral, $q_n$ must also divide the weight function.

Let $S(\omega) = \int_{-1}^{1} f_\omega(x)G(x)H(x)\pi(x) dx$, where $f_\omega(x) = \frac{\pi^2 x q_n(x)}{\omega \sin(\pi x / \omega)}$ and the factors $G$ and $H$ are chosen according to one of the two cases enumerated below.

Case A was examined in [14], while Case B is the one presented herein.

The calculations in case B are performed using formula (10) with $M = 1000$, whereas case A is worked out using Eq. (11). To compare with a Gauss quadrature formula of pure rational type we refer the reader to [22, 26] where other methods different from that presented here are used.

Tables 1 and 2 show the relative errors obtained when the $n$-point Gauss rule (5) is applied to $S(\omega)$ for two different values of $\omega$. The letter $d$ stands for the degree $d = 2n$ of polynomial (17). For both cases A and B, they have been computed $N = 2^{15} = 32768$ Chebyshev coefficients using FFT, with the exception of $G(t) = \sqrt{1 - t^2}$ whose coefficients are known explicitly and therefore it is enough to calculate a smaller quantity.
\[
\begin{array}{cccccc}
& d = 2n & A & B & & d = 2n & A & B \\
n & 3 & 6 & 1.1e - 04 & 1.1e - 04 & 6 & 12 & 5.9e - 08 & 1.2e - 11 \\
& 5 & 10 & 5.5e - 08 & 3.8e - 09 & 7 & 14 & 5.9e - 08 & 1.0e - 14 \\
& d = n & A & B & & d = n & A & B \\
n & 2 & 2 & 2.9e - 02 & 2.9e - 02 & 6 & 6 & 5.8e - 08 & 9.9e - 10 \\
& 4 & 4 & 1.2e - 05 & 1.2e - 05 & 8 & 8 & 5.9e - 08 & 6.7e - 15 \\
\end{array}
\]

Table 1: Example 4.1 with $\omega = 1.001$

\[
\begin{array}{cccccc}
& d = 2n & A & B & & d = 2n & A & B \\
n & 3 & 6 & 9.0e - 05 & 9.0e - 05 & 6 & 12 & 4.4e - 07 & 7.5e - 10 \\
& 5 & 10 & 4.3e - 07 & 2.3e - 09 & 7 & 14 & 4.4e - 07 & 7.6e - 10 \\
& d = n & A & B & & d = n & A & B \\
n & 2 & 2 & 2.6e - 02 & 2.6e - 02 & 6 & 6 & 4.4e - 07 & 4.3e - 11 \\
& 4 & 4 & 9.7e - 06 & 1.0e - 05 & 8 & 8 & 4.4e - 07 & 7.6e - 10 \\
\end{array}
\]

Table 2: Example 4.1 with $\omega = 1.0001$

4.2. Finite part integrals

The computation of (1) can be carried out after removing the main singularity, such as shown below.

\[
\int_{-1}^{1} \frac{F(t)w(t)dt}{(t-x)^2} = \int_{-1}^{1} E(x,t)w(t)dt + \Phi(w,x),
\]

where $w$ is a weight function on $(-1,1)$, $E(x,t)$ is defined in (3), and

\[
\Phi(w,x) = F(x) \int_{-1}^{1} \frac{w(t)dt}{(t-x)^2} + F'(x) \int_{-1}^{1} \frac{w(t)dt}{(t-x)}.
\]

Eq. (18) is the result of applying to (1) a technique based on the Taylor polynomial. It expresses a fairly general approach whose treatment depends to a large extent on the knowledge we have about $w(t)$. In principle, we can choose among several types of quadrature formulas to evaluate the integrals on the right side of Eq. (18). In fact, the final choice depends on the
characteristics that the two functions \( w(t) \) and \( E(x,t) \) have separately or jointly after multiplying one by the other. According to the previous sections, in what follows we assume that the density \( F(t) \) is nearly singular and \( w \equiv 1 \), although the case \( w = W \) can also be treated using our approach because \( \Phi(W,x) = 0 \). In particular, the following formula has been easily obtained calculating antiderivatives explicitly.

\[
\Phi(1, x) = -\frac{2F(x)}{1 - x^2} + F'(x) \log \left( \frac{1 - x}{1 + x} \right). \tag{19}
\]

If we are able to factorize \( F(t) = g(t)/h(t) \), where \( h(t) \) is positive, \( 1/h(t) \) is nearly-singular, and \( g \) is smooth, then we can write \( E(x,t) = f(x,t) \), where

\[
f(x,t) = \frac{(g(t)h(x) - g(x)h(t))h(x) - h(t)(t - x)\delta(x)}{h(x)^2}, \tag{20}
\]

and \( \delta(x) = h(x)g'(x) - h'(x)g(x) \).

Here we also assume that \( f(x,t)/(t - x)^2 \) is smooth for all \( x \in (-1, 1) \).

If the goal is to integrate with respect to a modification of the Chebyshev weight function of the first kind, then one may adopt the following expression for the integral on the right side of (18) when \( w \equiv 1 \) (cf. [14]).

\[
\int_{-1}^{1} E(x,t) dt = \int_{-1}^{1} \frac{f(x,t)K(t)W\pi(t)}{(t - x)^2} dt, \tag{21}
\]

where \( K(t) = \pi \sqrt{1 - t^2}/h(t) \). If \( w = W \), then we put \( K(t) = \pi/h(t) \).

In accordance with Elliott [19], the first stage of the method we are proposing here is to decompose \( K(t) \) into two factors, say \( K(t) = G(t)H(t) \), where \( G(t) = 1/h(t) \) and \( H(t) = \pi \sqrt{1 - t^2} \).

Gauss rules based on a \( GH \)-modification are really efficient when the integrand is parametric, a feature that the examples given below possess. Furthermore, this method allows to obtain good precision with few nodes.

Hereinafter, the calculation of Chebyshev coefficients have been performed using \( FFT \) with \( N = 2^{10} \). Moreover, when considering the \( GH \)-approach the modified moments are approximated using [10] with \( M = 10^3 \).

The examples shown in this part are based on the following integrals whose exact value has been calculated explicitly (cf. [11]).

\[
\int_{-1}^{1} \frac{dt}{(t - x)^2 \sqrt{\alpha^2 - t^2}}, \quad \alpha^2 > 1, \quad |x| < 1. \tag{22}
\]
4.2.1. $G$ vs. $GH$ ($\varepsilon = 0$)

Once we have obtained a suitable factorization $F = g/h$, we may construct the function $f(x,t)$ as indicated in (20). As for the integral (22) the choice is straightforward: $g \equiv 1$ and $h(t) = \sqrt{\alpha^2 - t^2}$.

**Example 4.2.** Both tables 3 and 4 show the results obtained when (22) is evaluated using the two options $A$ and $B$ below.

- $A$: $G(t) = \sqrt{1 - t^2}/\sqrt{\alpha^2 - t^2}$ and $H \equiv 1$.
- $B$: $G(t) = 1/\sqrt{\alpha^2 - t^2}$ and $H(t) = \sqrt{1 - t^2}$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$A$</th>
<th>$B$</th>
<th>$n$</th>
<th>$A$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.4e-01</td>
<td>3.4e-01</td>
<td>32</td>
<td>1.6e-05</td>
<td>8.7e-07</td>
</tr>
<tr>
<td>4</td>
<td>6.8e-02</td>
<td>6.8e-02</td>
<td>64</td>
<td>1.7e-05</td>
<td>3.6e-11</td>
</tr>
<tr>
<td>8</td>
<td>7.0e-03</td>
<td>7.1e-03</td>
<td>128</td>
<td>1.7e-05</td>
<td>1.4e-13</td>
</tr>
<tr>
<td>16</td>
<td>2.2e-04</td>
<td>2.4e-04</td>
<td>256</td>
<td>1.7e-05</td>
<td>2.0e-12</td>
</tr>
</tbody>
</table>

Table 3: Example 4.2 with $\alpha = 1.01$ and $x = 0.25$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$A$</th>
<th>$B$</th>
<th>$n$</th>
<th>$A$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.6e-00</td>
<td>1.6e-00</td>
<td>32</td>
<td>7.0e-04</td>
<td>8.8e-04</td>
</tr>
<tr>
<td>4</td>
<td>4.2e-01</td>
<td>4.2e-01</td>
<td>64</td>
<td>1.7e-04</td>
<td>1.6e-05</td>
</tr>
<tr>
<td>8</td>
<td>8.5e-02</td>
<td>8.6e-02</td>
<td>128</td>
<td>1.9e-04</td>
<td>1.8e-08</td>
</tr>
<tr>
<td>16</td>
<td>1.2e-02</td>
<td>1.2e-02</td>
<td>256</td>
<td>1.9e-04</td>
<td>8.3e-12</td>
</tr>
</tbody>
</table>

Table 4: Example 4.2 with $\alpha = 1.001$ and $x = 0.25$

It should be noted that when Gauss-Chebyshev quadrature formula applies to (22) with $\alpha = 1.01, 1.001, x = 0.25$ and $N = 2^{10}$ nodes, relative errors coincide with those produced by option $A$ in both tables 3 and 4 for $n \geq 32$, all of which is consistent with the results shown in [14].
4.2.2. Standard regularization vs. $\varepsilon$-regularization

In this part we keep the notation used in the previous sections.

Once we have selected $g(t)$ and $h(t)$, we put $G(t) = 1/h(t)$ and $H(t) = \pi \sqrt{1 - t^2}$. Let $f(x,t)$ be as in (20). From the two equations (15) and (21), it is obtained the following approximation formula.

$$\int_{-1}^{1} F(t)dt \approx \int_{-1}^{1} h(t)f(x,t(1-\varepsilon))G(t)H(t)W_{\pi}(t)dt + \Phi(1,x),$$

(23)

where $\Phi(1,x)$ is defined in (19) and $0 < \varepsilon < 1$.

Then, we first calculate the quadrature parameters of formula (5) to decide subsequently what the appropriate $\varepsilon$ value should be, always taking into account the distance between the singular point $x$ and the quadrature nodes.

Below, it is shown that the choice $\varepsilon = 10^{-6} \approx u^{1/3}/6$ produces more accurate results than those obtained by $\varepsilon = 0$, whenever $x \approx t$. Otherwise, it is immaterial whether one uses $\varepsilon$ small, e.g. $\varepsilon \leq 10^{-12}$, or $\varepsilon = 0$.

**Example 4.3.** Tables 5, 6 and 7 allow us to compare the standard regularization (column $B_0$), with the one based on the scheme (23) (column $B_\varepsilon$). These two approaches are used to evaluate (22) when the singular point is selected as $x = x_{n,n+1} + 10^{-15}$, where $n = 2r$ and $x_{n,r+1}$ is the $r+1$th node of the $n$th quadrature.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_\varepsilon$</th>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3.6e-00</td>
<td>4.2e-01</td>
<td>32</td>
<td>2.9e-02</td>
<td>1.3e-05</td>
</tr>
<tr>
<td>4</td>
<td>1.8e-00</td>
<td>1.2e-01</td>
<td>64</td>
<td>3.1e-03</td>
<td>2.6e-06</td>
</tr>
<tr>
<td>8</td>
<td>6.4e-01</td>
<td>1.7e-02</td>
<td>128</td>
<td>2.5e-04</td>
<td>6.1e-07</td>
</tr>
<tr>
<td>16</td>
<td>1.7e-01</td>
<td>6.4e-04</td>
<td>256</td>
<td>1.7e-05</td>
<td>1.5e-07</td>
</tr>
</tbody>
</table>

Table 5: Example 4.3 with $\varepsilon = 10^{-6}$, $x = x_{n,n/2+1} + 10^{-15}$, $\alpha = 1.01$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_\varepsilon$</th>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.4e+01</td>
<td>2.0e-00</td>
<td>32</td>
<td>4.3e-01</td>
<td>6.9e-03</td>
</tr>
<tr>
<td>4</td>
<td>7.0e-00</td>
<td>8.7e-01</td>
<td>64</td>
<td>1.0e-01</td>
<td>2.4e-04</td>
</tr>
<tr>
<td>8</td>
<td>3.2e-00</td>
<td>3.0e-01</td>
<td>128</td>
<td>1.4e-02</td>
<td>4.4e-05</td>
</tr>
<tr>
<td>16</td>
<td>1.3e-00</td>
<td>6.9e-02</td>
<td>256</td>
<td>1.4e-03</td>
<td>1.4e-05</td>
</tr>
</tbody>
</table>

Table 6: Example 4.3 with $\varepsilon = 10^{-6}$, $x = x_{n,n/2+1} + 10^{-15}$, $\alpha = 1.001$
Table 7: Example 4.3 with $\varepsilon = 10^{-6}$, $x = x_{n,n/2+1} + 10^{-15}$, $\alpha = 1.0001$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_{\varepsilon}$</th>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_{\varepsilon}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$5.1e+01$</td>
<td>$7.3e-00$</td>
<td>32</td>
<td>$2.4e-00$</td>
<td>$2.0e-01$</td>
</tr>
<tr>
<td>4</td>
<td>$2.3e+01$</td>
<td>$3.6e-00$</td>
<td>64</td>
<td>$9.3e-01$</td>
<td>$3.7e-02$</td>
</tr>
<tr>
<td>8</td>
<td>$1.2e+01$</td>
<td>$1.6e-00$</td>
<td>128</td>
<td>$2.8e-01$</td>
<td>$3.7e-03$</td>
</tr>
<tr>
<td>16</td>
<td>$5.5e-00$</td>
<td>$6.3e-01$</td>
<td>256</td>
<td>$5.5e-02$</td>
<td>$7.9e-04$</td>
</tr>
</tbody>
</table>

Table 8: Example 4.3 with $\varepsilon = 10^{-14}$, $x = 0.25$, $\alpha = 1.001$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_{\varepsilon}$</th>
<th>$n$</th>
<th>$B_0$</th>
<th>$B_{\varepsilon}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$1.6e-00$</td>
<td>$1.6e-00$</td>
<td>32</td>
<td>$8.8e-04$</td>
<td>$8.8e-04$</td>
</tr>
<tr>
<td>4</td>
<td>$4.2e-01$</td>
<td>$4.2e-01$</td>
<td>64</td>
<td>$1.6e-05$</td>
<td>$1.6e-05$</td>
</tr>
<tr>
<td>8</td>
<td>$8.6e-02$</td>
<td>$8.6e-02$</td>
<td>128</td>
<td>$1.8e-08$</td>
<td>$1.8e-08$</td>
</tr>
<tr>
<td>16</td>
<td>$1.2e-02$</td>
<td>$1.2e-02$</td>
<td>256</td>
<td>$8.3e-12$</td>
<td>$1.5e-11$</td>
</tr>
</tbody>
</table>

Table 8 indicates that when the distance between a given set of parameters and nodes is not small the good decision is to choose $\varepsilon$ very small or $\varepsilon = 0$.

5. Concluding remarks

Experimental results show that the method based on the substitution of the integration variable $t$ by $t(1 - \varepsilon)$ is able to mitigate the irregular behavior of the difference quotient of second order. It is a phenomenon that may occur when the collocation points are given in advance and the quadrature nodes are calculated subsequently. Once the distance between these two sets of points is known, we can properly choose the size of $\varepsilon$, provided the latter does not belong to the integrator.

When the density function misbehaves, we apply Gauss rules related to a suitable modification of the Chebyshev weight function. For numerical treatment, such modification should be decomposed conveniently into two factors, one of which is $\sqrt{1 - t^2}$ in many cases. The other factor must be extracted from the density function, an action that requires certain expertise. This procedure is quite general and can be used to compute efficiently the parameters of the quasi-rational quadrature formulas suggested by W. Gautschi.
Instead of the explicit formula for the derivative of the density function, one can use the corresponding symmetric difference quotient for calculations. If this replacement is conveniently carried out, then the accuracy of the results decreases slightly.

Acknowledgment

We thank the reviewers for their valuable suggestions and criticisms.

References


