

SIMPLE QUADRATURE FOR SINGULAR INTEGRALS

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ABSTRACT. In this note quadrature formulae for singular integrals are derived that retain the nice features of Gauss-Chebyshev quadrature, for example the easy to calculate weights and nodes. The reason for these new formulae lies in their application to a special method for solving singular integral equations, where such properties need to be preserved. The study shows that by subtracting the endpoint singularities, formulae converging to the desired integral are obtained. The rates of convergence are shown to depend on the exponents of the Gauss-Jacobi weight function. In practice, fast convergence is attained, giving full accuracy with a very small number of nodes, with execution times comparable to those of Gaussian quadrature.

1. Introduction. Quadrature formulae for integrals possessing a Cauchy principal value singularity have been investigated in the recent literature; and generally, Gaussian quadrature of some form has been used. In [10], for example, Gauss-Jacobi formulae have been derived for applications to singular integral equations. The problem of convergence of these rules has been resolved in [8]. A different approach has been considered in [4], where quadrature formulae have been derived so that the nodes coincide with the “practical” abscissae. Gauss type formulae, however, are not the only way of dealing with the problem [14].

The aim of this note is to derive formulae and convergence results for singular integrals with an approach similar to [4] where the nodes are prescribed to be “practical” abscissae. Here we also retain the simple weights of the classical Chebyshev quadrature.

The need for such formulae arises in applications to singular integral equations (SIE's) [18], where the integral is discretized using Gauss-Chebyshev quadrature, at the expense of accuracy, since the endpoint behavior of the solution is ignored. In this way it is possible to make

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use of known results on sums of zeros of Chebyshev polynomials [17] in the error analysis. The aim of our alternative algorithm is to obtain execution times comparable to the ordinary algorithm based on Gaussian quadrature, but simplifying the code considerably, since no subroutines for the calculation of quadrature nodes and weights are required. The error analysis of [18] for the negative index equation breaks down for index one, the reason being the presence of endpoint singularities. The present scheme is needed to accelerate the convergence of the scheme for the solution of the SIE with negative index, and to show convergence in the more physically interesting case of index 1. The rates of convergence of the proposed quadratures are shown to depend on the exponents of the Gauss-Jacobi weight. For a smooth integrand, very fast convergence is obtained, and double precision accuracy in our examples is reached by using 16 nodes, plus a small number of endpoint conditions, at most 10. The experiments show that the startup time for the endpoint interpolatory conditions is very small, and overall the execution time is comparable to the corresponding Gaussian quadrature. Another advantage of the present scheme is that it avoids the recalculation of the function evaluations at the nodes when doubling the system size.

We begin the note by giving the key to the error analysis of the formulae studied in the later sections. In Section 3 we study the formulae for a smooth integrand. These results are then extended to Cauchy principal value integrals in Section 4. In the last section we provide some illustrative examples of the proposed quadratures.

2. Preliminaries. In order to present the key idea underlying the paper, let us start by considering the problem of evaluating

$$(2.1) \quad I = \int_{-1}^1 w(x)f(x) dx,$$

where we assume

$$\int_{-1}^1 w(x) dx < \infty.$$

Here $f \in C^{m+\lambda}[-1, 1]$, $0 < \lambda \leq 1$, m a nonnegative integer, i.e., f has m continuous derivatives and the m -th derivative is a Hölder continuous function of exponent λ over $[-1, 1]$:

$$|f^{(m)}(x) - f^{(m)}(t)| \leq C|x - t|^\lambda, \quad x, t \in (-1, 1),$$

which is denoted by writing $f^{(m)} \in H_\lambda[-1, 1]$. The same notation will be used later, so that whenever $f \in C^\tau[-1, 1]$, $\tau \in \mathbf{R}^+$, we will always understand $f \in C^t[-1, 1]$, with $t \equiv [\tau]$, the integer part of τ , and $f^{(t)} \in H_{\tau-t}[-1, 1]$.

A quadrature formula can be constructed by replacing f , the smooth part of the integrand, with its Lagrange interpolatory polynomial $L_{n-1}(f, X, x)$ over a set of nodes $X = \{x_1, \dots, x_n\}$. The weights of the quadrature are easily obtained

$$(2.2) \quad \begin{aligned} Q_n &:= \int_{-1}^1 w(x) L_{n-1}(f, X, x) dx = \sum_{j=1}^n f(x_j) \int_{-1}^1 w(x) l_j(x) dx \\ &\equiv \sum_{j=1}^n w_j f(x_j). \end{aligned}$$

The quadrature error $\mathcal{R}_n(f) \equiv I - Q_n$ can be estimated using p_{n-1}^* , the best approximation polynomial of degree $n-1$ in the uniform norm, observing that it is interpolated exactly by the above Lagrange formula.

Let $\mathcal{E}_{n-1}(f)$ denote the best approximation error in the uniform norm, and let Π_{n-1} denote the set of polynomials of degree up to $n-1$, then

$$\mathcal{E}_{n-1}(f) = \|f - p_{n-1}^*\|_\infty \equiv \min_{p \in \Pi_{n-1}} \|f - p\|_\infty.$$

It then follows

$$\begin{aligned} |\mathcal{R}_n(f)| &= \left| \int_{-1}^1 w(x) [f(x) - p_{n-1}^*(x)] dx \right. \\ &\quad \left. + \int_{-1}^1 w(x) L_{n-1}(p_{n-1}^* - f, X, x) dx \right| \\ &\leq \mathcal{E}_{n-1}(f) \left[1 + \max_{-1 \leq x \leq 1} \sum_{j=1}^n |l_j(x)| \right] \int_{-1}^1 |w(x)| dx \\ &\equiv \mathcal{E}_{n-1}(f) [1 + \Lambda_n(X)] \int_{-1}^1 |w(x)| dx. \end{aligned}$$

Let us define $V_n \equiv \{t_1, \dots, t_n\}$, the set of the zeros of $T_n(x)$, the first kind Chebyshev polynomial of degree n . If $\Lambda(V_n)$ is the Lebesgue constant relative to the set V_n , then from [16, (1.3), p. 13],

$$\Lambda(V_n) \leq (2/\pi) \log(n) + 1, \quad n = 1, 2, \dots$$

Let $S_{n+1} \equiv \{s_0 \equiv 1, s_1, \dots, s_{n-1}, s_n \equiv -1\}$, where $s_j, j = 1, \dots, n-1$, denote the zeros of $U_{n-1}(x)$, the second kind Chebyshev polynomial of degree $n-1$. It has been shown that $\Lambda(S_{n+1}) \leq \Lambda(V_n)$, so that a result similar to the above holds for $X \equiv S_{n+1}$, [6, (4.6) and (5.1)].

Let us denote by $\omega(f, \delta)$ the modulus of continuity of the function f . The following theorem is well known [11, Theorem VIII, p. 18]. It can be stated as follows:

Theorem. *If $f \in C^{m+\lambda}[-1, 1]$, with m and λ defined above, then for every $n > m$, there is a polynomial of degree n , $P_n(x)$, such that, for every $x \in [-1, 1]$,*

$$|f(x) - P_n(x)| \leq Cn^{-m}\omega(f^{(m)}, 2/(n-m)).$$

This result simply estimates the best approximation error in the uniform norm. Let us observe that the modulus of continuity can be estimated in terms of the exponent of the Hölder class to which the function belongs, [4]. We then have, for $X \equiv V_n$ or $X \equiv S_{n+1}$,

$$\begin{aligned} |\mathcal{R}_n(f)| &\leq C_1 \mathcal{E}_{n-1}(f)[1 + \Lambda(X)] \\ (2.3) \quad &\leq C_2 n^{-m} \omega(f^{(m)}, 2/(n-m)) \log(n) \\ &\leq C_3 n^{-(m+\lambda)} \log(n) \leq C_4 n^{-(m+\lambda)+\varepsilon}, \end{aligned}$$

with $\varepsilon > 0$ arbitrarily small. In summary,

Proposition 1. *For $w(x) = (1-x^2)^{-1/2}$, the rate of convergence of the quadrature formula (2.2) is determined by (2.3), in the two cases corresponding to Gauss-Chebyshev quadrature, $X \equiv V_n$, $x_k = t_k$, $w_k = n^{-1}$, $k = 1, \dots, n$, and to Lobatto-Chebyshev quadrature, $X \equiv S_{n+1}$, $x_j = s_j$, $w_j = n^{-1}$, $j = 0, 1, \dots, n$.*

Remark. From this statement the fundamental role played by the degree of smoothness of f is evident. An integration rule will be constructed by suitably modifying the integrand so as to apply Gauss-Chebyshev or Lobatto-Chebyshev quadrature. Throughout the paper the result will be used to obtain convergence rates by determining how

many continuous derivatives the “modified” integrand possesses and in which Hölder class the highest continuous derivative lies.

To obtain asymptotic estimates on the rates of convergence, the remainder of the quadrature must be rewritten as a contour integral. From (2.2), the weights can be explicitly rewritten by letting

$$p_n(x) = \prod_{j=1}^n (x - x_j),$$

to obtain

$$(2.4) \quad w_j = [p'_n(x_j)]^{-1} \int_{-1}^1 w(x) p_n(x) (x - x_j)^{-1} dx.$$

The “second kind functions” are defined as follows [2]:

$$(2.5) \quad q_n(z) := \int_{-1}^1 w(x) p_n(x) (z - x)^{-1} dx, \quad z \notin [-1, 1].$$

From Cauchy’s formula, if C is a contour containing the interval $[-1, 1]$ in its interior, with no singularity of f lying on it or in its interior, we can write

$$(2.6) \quad \int_{-1}^1 f(t) w(t) dt = (2\pi i)^{-1} \int_C f(z) \int_{-1}^1 w(t) (z - t)^{-1} dt dz.$$

Define $\hat{P}(z)$ by

$$\hat{P}(z) := [p_n(z)]^{-1} \int_{-1}^1 [p_n(z) - p_n(t)] w(t) (z - t)^{-1} dt, \quad z \notin [-1, 1].$$

Then from (2.4) w_j is the residual of $\hat{P}(z)$ at $z \equiv x_j$, so that

$$(2.7) \quad \sum_{j=1}^n w_j f(x_j) = \sum_{j=1}^n \text{Res}(\hat{P}f, x_j) = (2\pi i)^{-1} \int_C f(z) \hat{P}(z) dz.$$

On using the definition of \hat{P} in (2.7), from (2.6) and the definition of $\mathcal{R}_n(f)$, it follows

$$(2.8) \quad \mathcal{R}_n(f) = (2\pi i)^{-1} \int_C f(z)q_n(z)/p_n(z) dz.$$

We will use this formula together with the representations for $q_n(z)/p_n(z)$ provided by [5], which hold for any $z \in \mathbf{C}$, for $p_n(z)$ being the first and second kind Chebyshev polynomials. In the former case, from [5, (A.4)], we have

$$(2.9) \quad q_n(z)/T_n(z) = 2\pi(z^2 - 1)^{-1/2} \{ [z + (z^2 - 1)^{1/2}]^{2n} + 1 \}^{-1}.$$

For Lobatto-Chebyshev quadrature, notice that $p_n(x)$ in (2.5) should be replaced by the polynomial $(1 - x^2)U_{n-1}(x)$. Let $q_{n+1}^{LC}(z)$ denote the second kind function arising from these polynomials. It is easily seen that, denoting by $q_{n-1}^{2K}(z)$, the same function arising from the second kind Chebyshev polynomials, i.e., from the replacement of p_n in formula (2.5) by the polynomial U_{n-1} , we have

$$\begin{aligned} q_{n+1}^{LC}(z) &\equiv \int_{-1}^1 U_{n-1}(x)(1 - x^2)(z - t)^{-1}(1 - x^2)^{-1/2} dt \\ &\equiv \int_{-1}^1 U_{n-1}(x)(z - t)^{-1}(1 - x^2)^{1/2} dt \equiv q_{n-1}^{2K}(z). \end{aligned}$$

We can then use (A.5) of [5] for $q_{n-1}^{2K}(z)/U_{n-1}(z)$ to get

$$(2.10) \quad q_{n+1}^{LC}(z)(z^2 - 1)^{-1}/U_{n-1}(z) \equiv 2\pi(z^2 - 1)^{-1/2} \{ [z + (z^2 - 1)^{1/2}]^{2n} - 1 \}^{-1}.$$

Since these functions have branch points at ± 1 , we choose the cuts to be from 1 to infinity along the positive real axis, and symmetrically on the negative real axis, i.e., we assume

$$(2.11) \quad -\pi < \arg(z + 1) < \pi, \quad 0 < \arg(z - 1) < 2\pi.$$

In the rest of the paper, the following quantities will be used

$$(2.12) \quad \begin{aligned} \alpha &= \gamma + 1/2, & \beta &= \delta + 1/2, \\ \lambda &= \alpha + r + 1, & \zeta &= \beta + l + 1, \\ \tau &= \min(\lambda, \zeta), & \xi &= \tau - 1. \end{aligned}$$

3. Smooth integrands. Let us define $\rho_{\delta\gamma}(x) = (1+x)^\delta(1-x)^\gamma$. The integral under consideration in this section can be written as

$$(3.1) \quad I = \frac{1}{\pi} \int_{-1}^1 \rho_{\delta\gamma}(x)g(x) dx$$

with $g(x)$ smooth in $[-1, 1]$. The integrability conditions require that $\gamma, \delta > -1$; and the worst case is $-1 < \gamma, \delta < 0$, for which the integrand is unbounded at both endpoints. Introducing the Chebyshev weight of the first kind, we can rewrite (3.1) as

$$(3.2) \quad I = \frac{1}{\pi} \int_{-1}^1 \rho_{\beta\alpha}(x)g(x) \frac{dx}{\sqrt{1-x^2}}.$$

Let $p_{\ell r}(x)$ represent the polynomial of degree $\leq \ell+r+1$ interpolating $g(x)$ and its first ℓ derivatives at -1 , and interpolating g and its first r derivatives at 1 . Explicitly, letting $D^j \equiv d^j/dx^j$,

$$(3.3) \quad p_{\ell r}(x) = \sum_{i=0}^{\ell} L_i^{\ell r}(x)g^{(i)}(-1) + \sum_{i=0}^r R_i^{\ell r}(x)g^{(i)}(1),$$

where $L_i^{\ell r}(x)$ and $R_i^{\ell r}(x)$ satisfy

$$(3.4) \quad \begin{aligned} (D^q L_i^{\ell r})(-1) &= \delta_{iq} \quad i, q = 0, 1, \dots, \ell, \\ (D^q L_i^{\ell r})(1) &= 0, \quad i = 0, 1, \dots, \ell, \quad q = 0, 1, \dots, r, \\ (D^q R_i^{\ell r})(-1) &= 0 \quad i = 0, 1, \dots, r, \quad q = 0, 1, \dots, \ell, \\ (D^q R_i^{\ell r})(1) &= \delta_{iq}, \quad i, q = 0, 1, \dots, r. \end{aligned}$$

The polynomials $L_i^{\ell r}(x)$, $i = 0, 1, \dots, \ell$, and $R_j^{\ell r}(x)$, $j = 0, 1, \dots, r$, can be written in terms of powers of $(1-x)$ and $(1+x)$ as follows:

$$(3.5) \quad \begin{aligned} L_i^{\ell r}(x) &= (1-x)^{r+1} \sum_{j=0}^{\ell} l_{ij}^{\ell r} (1+x)^j, \quad i = 0, \dots, \ell, \\ R_i^{\ell r}(x) &= (1+x)^{\ell+1} \sum_{j=0}^r r_{ij}^{\ell r} (1-x)^j, \quad i = 0, \dots, r. \end{aligned}$$

Lemma. *The coefficients in the above expressions have the explicit form*

$$(3.6) \quad \begin{aligned} l_{ij}^{\ell r} &= \begin{cases} 0 & \text{for } i > j \\ 2^{-(r+j+1-i)}/i! \binom{r+j-i}{r} & \text{for } i \leq j \end{cases} \\ r_{ij}^{\ell r} &= \begin{cases} 0 & \text{for } i > j \\ (-1)^i 2^{-(\ell+j+1-i)}/i! \binom{\ell+j-i}{\ell} & \text{for } i \leq j. \end{cases} \end{aligned}$$

Proof. We only sketch the proof of the first claim. Omitting the superscripts, from (3.5) for $q < i$, we have a homogeneous nonsingular triangular system, so that $l_{i,j} = 0$, $j = 0, 1, \dots, i-1$. Using this fact for $q = i$, we immediately have $l_{ii} = 1/i! 2^{-r-1}$, verifying (3.6). By induction, we then need to show that

$$\sum_{k=0}^q (-1)^k \binom{q}{k} (r+1)_k 2^{r+1-k} l_{i,q-k} (q-k)! = 0.$$

Rewriting, using the inductive assumption, the previous result, and (3.6), the claim is then reduced to showing that

$$\sum_{k=0}^{q-i} (-1)^{k+1} \binom{r+1}{k} \binom{r+q-k-i}{r} = 0.$$

The identity

$$\binom{r+1}{k} \binom{r+q-k-i}{r} = \binom{r+q-i}{r+k} \binom{r+k}{r}$$

is verified since the left hand side counts the number of ways of selecting k objects from a set of $r+1$, then adding to the set another $q-i$ objects and selecting additional r . The same result is obtained by immediately adding to the box the $q-i-1$ extra objects, selecting $r+k$ of them and, from these, then selecting a subset of r elements. The right hand side counts the number of ways of proceeding in this way. Using the

identity we verify the former formula, since it reduces to $(1-x)^{q-i}$ evaluated at $x=1$. \square

Now let $H_{\ell r}(x) \equiv \rho_{\beta\alpha}(x)[g(x) - p_{\ell r}(x)]$. Subtracting out the endpoint singularities, the integral I can be rewritten as

$$(3.7) \quad I = \frac{1}{\pi} \int_{-1}^1 H_{\ell r}(x) \frac{dx}{\sqrt{1-x^2}} + \frac{1}{\pi} \int_{-1}^1 \rho_{\delta\gamma}(x) p_{\ell r}(x) dx.$$

Gauss-Chebyshev quadrature can now be applied to the first integral. The second term can be evaluated analytically by means of [9, (3.196.3), p. 285]

$$(3.8) \quad E(\nu, \mu) \equiv \frac{1}{\pi} \int_{-1}^1 (1-x)^\mu (1+x)^\nu dx = \frac{2^{\mu+\nu+1}}{\pi} \frac{\Gamma(\mu+1)\Gamma(\nu+1)}{\Gamma(\mu+\nu+2)},$$

$\operatorname{Re}(\mu), \operatorname{Re}(\nu) > 0.$

We obtain in this way an approximate value for I , which we denote by $Q_n^{\ell r}$, since it is obtained with ℓ, r -type endpoint interpolation and n quadrature nodes. Then

$$(3.9) \quad Q_n^{\ell r} := \frac{1}{n} \sum_{k=1}^n H_{\ell r}(t_k) + \sum_{i=0}^{\ell} g^{(i)}(-1) \sum_{j=0}^{\ell} l_{ij}^{\ell r} E(j+\delta, r+1+\gamma) \\ + \sum_{i=0}^r g^{(i)}(1) \sum_{j=0}^r r_{ij}^{\ell r} E(\ell+1+\delta, j+\gamma).$$

Alternatively, Lobatto-Chebyshev quadrature can be used. Proceeding as above, we are led to the quadrature which we denote by $\hat{Q}_{n+1}^{\ell r}$:

$$(3.10) \quad \hat{Q}_{n+1}^{\ell r} := \frac{1}{n} \sum_{k=0}^n H_{\ell r}(s_k) + \sum_{i=0}^{\ell} g^{(i)}(-1) \sum_{j=0}^{\ell} l_{ij}^{\ell r} E(j+\delta, r+1+\gamma) \\ + \sum_{i=0}^r g^{(i)}(1) \sum_{j=0}^r r_{ij}^{\ell r} E(\ell+1+\delta, j+\gamma),$$

where the terms for $k = 0$ and $k = n$ in the first sum are halved.

To determine the rate of convergence of these formulae, use Proposition 1. We then have

Proposition 2. *The error in the quadrature formulae (3.9) and (3.10) converges at worst as*

$$(3.11) \quad |\mathcal{R}_n(H_{\ell_r})| \leq Cn^{-\tau+\varepsilon}, \quad |\hat{\mathcal{R}}_n(H_{\ell_r})| \leq \hat{C}n^{-\tau+\varepsilon},$$

with $\varepsilon > 0$ arbitrarily small, C, \hat{C} being constants, where we recall that $\tau = \min(\lambda, \zeta)$.

Proof. We need only to determine the behavior of $H_{\ell_r}(x)$ near each endpoint, since inside the interval $(-1, 1)$ H_{ℓ_r} is smooth; by using Taylor's formula, it is easily seen that it behaves as $(1-x)^\lambda$ near $x = 1$ and as $(1+x)^\zeta$ near $x = -1$, with $\alpha, \beta > -1/2$. It follows that $H_{\ell_r} \in C^\tau[-1, 1]$. The claim follows from Proposition 1. \square

An improvement can be obtained by using an asymptotic analysis, following [2, 5]. The function $\rho_{\beta\alpha}(x)$, from which $H_{\ell_r}(x)$ depends, is extended to the complex plane by the cuts (2.11). We specialize now the contour C of (2.8) by taking it to be made by two arcs of the circle in the complex plane $\operatorname{Re} e^{i\theta}$, $\varphi \leq \theta \leq \pi - \varphi$, $\varphi = \arcsin(\eta/R)$, $\eta > 0$ small, and $\pi + \varphi \leq \theta \leq 2\pi - \varphi$, $R > 1$, by two arcs of circle of radius $\varepsilon < 1$ around the points -1 and 1 , $1 + \varepsilon e^{i\theta}$, $\psi \leq \theta \leq 2\pi - \psi$, and $-1 + \varepsilon e^{i\theta}$, $\pi - \psi < \theta \leq -\pi + \psi$, $\psi = \arcsin(\eta/\varepsilon)$, and by the portions of the real axis joining these circles, described once in each sense, i.e., the four segments $[1 + \varepsilon + i\eta, R + i\eta]$, $[-R + i\eta, -1 - \varepsilon + i\eta]$, $[-1 - \varepsilon - i\eta, -R - i\eta]$, $[R - i\eta, 1 + \varepsilon - i\eta]$. The result can be stated as follows.

Proposition 3. *If $c(H_{\ell_r}, \tau)$ denotes a constant depending on the integrand but independent of n , with τ as defined in (2.12), for the quadrature formulae (3.9) and (3.10), we have asymptotically,*

$$(3.12) \quad \mathcal{R}_n(H_{\ell_r}) \cong c(H_{\ell_r}, \tau)n^{-2\tau-1}, \quad \hat{\mathcal{R}}_n(H_{\ell_r}) \cong \hat{c}(H_{\ell_r}, \tau)n^{-2\tau-1}.$$

Proof. From the definition of $H_{\ell r}$, asymptotically as $z \rightarrow \pm 1$, [2],

$$(3.13) \quad H_{\ell r}(z) \cong (z+1)^\zeta (1-z)^\lambda.$$

Since the contributions of the segments of the contour C are the only ones that are not negligible in the limit as $R \rightarrow \infty$ and $\varepsilon \rightarrow 0$, from (2.8) for $\eta > 0$, we obtain

$$\begin{aligned} \mathcal{R}_n(H_{\ell r})(2\pi i)^{-1} & \left[\int_{1+\varepsilon+i\eta}^{R+i\eta} + \int_{-R+i\eta}^{-1-\varepsilon+i\eta} + \int_{-1-R-i\eta}^{-R-i\eta} \right. \\ & \left. + \int_{R-i\eta}^{1+\varepsilon-i\eta} \right] H_{\ell r}(z) q_n(z)/p_n(z) dz. \end{aligned}$$

Let

$$\Psi(x) \equiv \begin{cases} \{[x + (x^2 - 1)^{1/2}]^{2n} + 1\}^{-1}, & \text{if Gauss-Chebyshev quadrature is used} \\ \{[x + (x^2 - 1)^{1/2}]^{2n} - 1\}^{-1}, & \text{if Lobatto-Chebyshev quadrature is used.} \end{cases}$$

As $\varepsilon, \eta \rightarrow 0$, $R \rightarrow \infty$, using (3.13), (2.9) and (2.10), the expression for the remainder becomes

$$\begin{aligned} \mathcal{R}_n(H_{\ell r}) & = 2 \sin(\pi\lambda) \int_1^\infty (1+x)^{\delta+\ell+1} (x-1)^{\gamma+r+1} \Psi(x) dx \\ & + (-1)^{\gamma+\delta+r+\ell} 2 \sin(\pi\zeta) \\ & \cdot \int_1^\infty (1+x)^{\gamma+r+1} (x-1)^{\delta+\ell+1} \Psi(-x) dx. \end{aligned}$$

Use now the substitution $x = \cos h\theta$. Notice that $\Psi(\cos h\theta) \cong (\cosh \theta)^{-2n} \cong e^{-2n\theta}$, so that for large θ the integrand is negligible. Thus the major contribution of the integrand is near the origin. These considerations make the replacement $1 + \cos h\theta \cong 2 + \theta^2/2 \cong 2$ permissible. We finally obtain the estimate

$$\begin{aligned} \mathcal{R}_n(H_{\ell r}) & \cong 2^{\delta+\ell+1-\gamma-r} \sin(\pi\lambda) \int_0^\infty \theta^{2\gamma+2r+3} e^{-2n\theta} d\theta \\ & + (-1)^{\gamma+\delta+r+\ell} 2^{\gamma+r+1-\delta-\ell} \sin(\pi\zeta) \int_0^\infty \theta^{2\delta+2\ell+3} e^{-2n\theta} d\theta. \end{aligned}$$

Letting $t = n\theta$, the claim finally follows. \square

4. Cauchy principal value integrals. The integral considered in this section is

$$(4.1) \quad I(a) = \frac{1}{\pi} \int_{-1}^1 \rho_{\delta\gamma}(x) \frac{g(x)}{x-a} dx,$$

where the symbol on the right hand side represents the Cauchy principal value and g is smooth in $[-1, 1]$. It can be rewritten as follows:

$$(4.2) \quad I(a) = \frac{1}{\pi} \int_{-1}^1 \rho_{\beta\alpha}(x) \frac{g(x)}{x-a} \frac{dx}{\sqrt{1-x^2}}.$$

For SIE's, an important quantity which ties the physics of the underlying phenomenon with the mathematical properties of the solution is given by the index χ , defined in terms of the coefficients of the equation, see [18]. For equations with constant coefficients, the index can be shown to be $\chi = -(\gamma + \delta)$ and always to attain the values $-1, 0$ or 1 . For the negative index -1 , the function $\rho_{\beta\alpha}(x)$ is bounded at the endpoints. After adding and subtracting $g(a)$ from $g(x)$, the integral is split and the Cauchy principal value is thus replaced by a bounded term, using the smoothness assumption on g . Gauss-Chebyshev quadrature can thus be applied. For the SIE discretized in this way, convergence is ensured. For the details on the procedure and on the results, see [18]. The same situation occurs if the index is zero and $-1/2 \leq \gamma \leq 0$ or $-1/2 \leq \delta \leq 0$. The remaining cases lead to a function $\rho_{\beta\alpha}(x)$ which is unbounded at least at one of the two endpoints; using the above analysis, not even convergence can be obtained. The worst case arises for $-1 < \gamma \leq -1/2 \leq \delta < 0$, or for the symmetric situation obtained by exchanging δ and γ . In such situations, the behavior of the weight function must explicitly be taken into account, before being able to apply the quadrature. The following scheme is proposed as a corrective. It is our hope that it will help in solving SIE's of positive index and, perhaps, lead to a viable speedup also for the scheme already proposed for negative index SIE's.

Let us define

$$(4.3) \quad \sigma_{\ell r}(x) = \rho_{\beta\alpha}(x)[g(x) - p_{\ell r}(x)].$$

Observe that $\sigma_{\ell r}$ is smooth inside $(-1, 1)$, and near the endpoints,

$$\sigma_{\ell r}(x) \cong C(1-x)^\lambda, \quad \sigma_{\ell r}(x) \cong C(1+x)^\zeta,$$

so that $\sigma_{\ell r} \in C^\tau[-1, 1]$, provided that g belongs at least to the same class. The integral can then be calculated by rewriting it as follows:

$$(4.4) \quad \begin{aligned} I(a) = & \frac{1}{\pi} \int_{-1}^1 [\sigma_{\ell r}(x) - \sigma_{\ell r}(a)](x-a)^{-1} \frac{dx}{\sqrt{1-x^2}} \\ & + \pi^{-1} \int_{-1}^1 \rho_{\delta\gamma}(x) p_{\ell r}(x)/(x-a) dx, \end{aligned}$$

where we have used the fact that

$$\int_{-1}^1 (x-a)^{-1} \frac{dx}{\sqrt{1-x^2}} = 0.$$

On the first integral, Gauss-Chebyshev quadrature can be applied, and the second integral can be evaluated by means of the following formula [9 (3.228.3), p. 290]

$$(4.5) \quad \begin{aligned} E^*(\nu, \mu, a) &= \int_{-1}^1 \frac{(1+x)^\nu (1-x)^\mu}{x-a} dx \\ &= (1+a)^\nu (1-a)^\mu \cot(\pi(\mu+1)) \\ &\quad - 2^{\mu+\nu} B(\mu, \nu+1) {}_2F_1(-\mu-\nu, 1; 1-\mu; (1-a)/2), \\ &\quad \operatorname{Re} \mu, \operatorname{Re} \nu > 0, -1 < a < 1. \end{aligned}$$

Define the following function:

$$(4.6) \quad h_{\ell r}(x) = \begin{cases} [\sigma_{\ell r}(x) - \sigma_{\ell r}(a)](x-a)^{-1}, & \text{if } x \neq a \\ \sigma'_{\ell r}(a), & \text{if } x = a. \end{cases}$$

Thus $h_{\ell r}(x) \in C^\xi(-1, 1)$. Then, proceeding similarly to the previous section, we can introduce the quadrature $Q_n^{\ell r}(a)$, obtained by ℓ, r -type endpoint interpolation on the singular integral, followed by Gauss-Chebyshev quadrature

$$(4.7) \quad \begin{aligned} Q_n^{\ell r}(a) := & \frac{1}{n} \sum_{k=1}^n h_{\ell r}(t_k) + \sum_{i=0}^{\ell} g^{(i)}(-1) \sum_{j=0}^{\ell} l_{ij}^{\ell r} E^*(j+\delta, r+1+\gamma, a) \\ & + \sum_{i=0}^r g^{(i)}(1) \sum_{j=0}^r r_{ij}^{\ell r} E^*(\ell+1+\delta, j+\gamma, a). \end{aligned}$$

An alternative procedure is to repeat the argument followed by Lobatto-Chebyshev quadrature, thus obtaining the quadrature denoted by $\hat{Q}_{n+1}^{\ell r}(a)$:

$$(4.8) \quad \begin{aligned} \hat{Q}_{n+1}^{\ell r}(a) : &= \frac{1}{n} \sum_{k=0}^n h_{\ell r}(s_k) + \sum_{i=0}^{\ell} g^{(i)}(-1) \sum_{j=0}^{\ell} l_{ij}^{\ell r} E^*(j + \delta, r + 1 + \gamma, a) \\ &+ \sum_{i=0}^r g^{(i)}(1) \sum_{j=0}^r r_{ij}^{\ell r} E^*(\ell + 1 + \delta, j + \gamma, a). \end{aligned}$$

We then have

Proposition 4. *The quadrature formulae (4.7) and (4.8) for the Cauchy principal value integral (4.2) converge at worst as*

$$(4.9) \quad |\mathcal{R}_n(h_{\ell r})| \leq Cn^{-\xi+\varepsilon}, \quad |\hat{\mathcal{R}}_n(h_{\ell r})| \leq \hat{C}n^{-\xi+\varepsilon},$$

with $\varepsilon > 0$ arbitrarily small. Asymptotically, a better estimate is given by

$$(4.10) \quad \mathcal{R}_n(h_{\ell r}) \cong c(h_{\ell r}, \xi)n^{-2\xi-1}, \quad \hat{\mathcal{R}}_n(h_{\ell r}) \cong \hat{c}(h_{\ell r}, \xi)n^{-2\xi-1},$$

where we recall $\xi = \min(\lambda, \zeta) - 1$.

Proof. The first claim follows from Proposition 1, since $\sigma_{\ell r} \in C^\xi[-1, 1]$, by repeating the arguments of Proposition 2. For the asymptotic estimate, proceed as in Proposition 3, with $H_{\ell r}$ replaced by $h_{\ell r}$, observing that in this case we have $h_{\ell r} \cong (1+x)^\zeta(1-x)^\lambda$. \square

In the particular case that a is a zero of a Chebyshev polynomial of the second kind, $U_n(a) = 0$ for some n ; then also $U_q(a) = 0$ for $q = n \cdot 2^m$ and $m = 1, 2, \dots$. The remark following (2.10) of [8] on the convergence to zero of the quadrature error $\mathcal{R}_n(h_{\ell r})$ can then be applied so that the rate of convergence will be τ rather than ξ . Using results on the sum of zeros of Chebyshev polynomials of first and second kind of [17],

$$\sum_{k=1}^n \frac{1}{t_k - s_j} = 0, \quad j = 1, \dots, n-1,$$

we can simplify (4.7) as follows:

(4.11)

$$Q_n^{\ell r}(a) = \frac{1}{n} \sum_{k=1}^n \frac{\sigma_{\ell r}(t_k)}{t_k - a} + \sum_{i=0}^{\ell} g^{(i)}(-1) \sum_{j=0}^{\ell} l_{ij}^{\ell r} E^*(j + \gamma, r + 1 + \delta, a) \\ + \sum_{i=0}^r g^{(i)}(1) \sum_{j=0}^r r_{ij}^{\ell r} E^*(\ell + 1 + \gamma, j + \delta, a).$$

5. Numerical experiments and discussion. We performed some experiments on an 80386-based machine. In all the examples, the smooth part of the integrand is $\exp(x)$. We provide for comparison the value and the execution time for the corresponding Gaussian quadrature. We give the time for Gaussian quadrature for the minimum number of nodes that gives double precision accuracy, and also for a larger number of nodes. We do this because to obtain an accurate answer in solving an SIE, a system of about that size must be solved. Also we give the startup time to calculate the quantities $E(\nu, \mu)$ and $E^*(\nu, \mu, a)$ for evaluating the interpolatory polynomials. This time added to the execution time of each run is seen to be comparable to the time needed by Gaussian quadrature. We show the results obtained by running some different cases. By increasing the degree of endpoint interpolation, the rate of convergence is increased at the expense of execution time and of the complexity of the code. We found that a 4,4-type formula is satisfactory from both points of view.

Even though the integrand does not satisfy the hypotheses of the asymptotic analysis, we see that the actual convergence rate is close to the theoretical one. At first, it is usually larger than the theoretical value, then decreasing with the increase of n . The final values shown in the tables do not show any improvement since they are clearly affected by round-off errors. However, this is easily explained by observing that we are down to machine accuracy, by counting the digits of the result. Even Gaussian quadrature exhibits oscillations in the next to the last digit in Table 1.

Table 1 illustrates Section 3 using formula (3.9). The results exhibit fast convergence, even when the endpoint singularities approach -1 . In Table 2, we consider the Cauchy principal value integral. The "collocation point" a is chosen to be very close to the endpoint, to show

the behavior of quadrature (4.7) on this badly behaved case, when the endpoint singular behavior is coupled with the Cauchy principal value singularity. This must be analyzed since, in case of an integral equation, when the size of the system grows large, the collocation points approach the endpoints. Even in this situation the proposed algorithm exhibits fast convergence. It is our hope that a scheme for the solution of singular integral equations with variable coefficients can be constructed using the method presented here. This has the advantage of avoiding the construction of the nonclassical weights and nodes required by the integral. Should a second run with twice as many nodes be required, another advantage is the reuse of previous function evaluations at the old nodes, if the Lobatto-Chebyshev scheme is used.

TABLE 1.

$g(x) = \exp(x)$, $\gamma = -.97600$, $\delta = -.98900$, startup time = 0.05

Gaussian quadrature:

8 nodes, value 74.02104606681937; time used = .06

35 nodes, value 74.02104606681917; time used = .44

		$\ell = 2, r = 2$	$2\tau + 1 = 6.022$
time	n	$\mathcal{R}_n(H_{\ell r})$	$\log \mathcal{R}_n(H_{\ell r})/\mathcal{R}_{2n}(H_{\ell r}) /\log(2)$
.00	2	-.751E-03	
.00	4	.549E-05	7.09
.00	8	.468E-07	6.87
.05	16	.636E-09	6.20
.06	32	.936E-11	6.09
.11	64	.568E-13	7.36
.22	128	-.852E-13	-.58
		$\ell = 3, r = 3$	$2\tau + 1 = 8.022$
time	n	$\mathcal{R}_n(H_{\ell r})$	$\log \mathcal{R}_n(H_{\ell r})/\mathcal{R}_{2n}(H_{\ell r}) /\log(2)$
.00	2	.165E-04	
.05	4	.260E-06	5.98
.00	8	.171E-09	10.57
.06	16	.412E-12	8.70
.11	32	-.852E-13	2.27

TABLE 1 (continued).

$\ell = 3, r = 4$				$2\tau + 1 = 8.022$
time	n	$\mathcal{R}_n(H_{\ell r})$	$\log \mathcal{R}_n(H_{\ell r})/\mathcal{R}_{2n}(H_{\ell r}) /\log(2)$	
.05	2	-.202E-05		
.00	4	-.410E-07	5.63	
.06	8	-.185E-10	11.11	
.11	16	-.142E-12	7.03	
.11	32	-.852E-13	.74	
$\ell = 2, r = 4$				$2\tau + 1 = 6.022$
time	n	$\mathcal{R}_n(H_{\ell r})$	$\log \mathcal{R}_n(H_{\ell r})/\mathcal{R}_{2n}(H_{\ell r}) /\log(2)$	
.00	2	-.132E-04		
.00	4	.469E-06	4.82	
.06	8	.204E-08	7.84	
.05	16	.262E-10	6.29	
.11	32	.312E-12	6.39	
.22	64	-.710E-13	2.14	
.44	128	-.852E-13	-.26	
$\ell = 4, r = 4$				$2\tau + 1 = 10.022$
time	n	$\mathcal{R}_n(H_{\ell r})$	$\log \mathcal{R}_n(H_{\ell r})/\mathcal{R}_{2n}(H_{\ell r}) /\log(2)$	
.00	2	-.192E-06		
.06	4	-.121E-07	3.99	
.05	8	.710E-12	14.06	
.06	16	-.710E-13	3.32	
.22	32	-.852E-13	-.26	

TABLE 2.

$g(x) = \exp(x)$, $a = .99$, $\gamma = -.9900$, $\delta = -.0100$, startup time = 0.05

Gaussian quadrature:

7 nodes, value 25784.92851530243; time used = .05

35 nodes, value 25784.92851530243; time used = .50

		$\ell = 2, r = 3$	$2\xi + 1 = 5.98$
time	n	$\mathcal{R}_n(h_{\ell r})$	$\log \mathcal{R}_n(h_{\ell r})/\mathcal{R}_{2n}(h_{\ell r}) /\log(2)$
.00	2	-.116E-03	
.06	4	.118E-05	6.62
.05	8	.723E-08	7.36
.06	16	.618E-10	6.87
.16	32	-.727E-11	3.09
		$\ell = 3, r = 3$	$2\xi + 1 = 6.02$
time	n	$\mathcal{R}_n(h_{\ell r})$	$\log \mathcal{R}_n(h_{\ell r})/\mathcal{R}_{2n}(h_{\ell r}) /\log(2)$
.00	2	-.921E-05	
.00	4	.500E-06	4.20
.11	8	.172E-08	8.18
.11	16	.727E-11	7.89
.22	32	-.727E-11	.00
		$\ell = 3, r = 4$	$2\xi + 1 = 7.98$
time	n	$\mathcal{R}_n(h_{\ell r})$	$\log \mathcal{R}_n(h_{\ell r})/\mathcal{R}_{2n}(h_{\ell r}) /\log(2)$
.05	2	.202E-05	
.00	4	.218E-07	6.53
.11	8	.145E-10	10.55
.17	16	-.727E-11	1.00

TABLE 2 (continued).

		$\ell = 2, r = 4$	$2\xi + 1 = 5.98$
time	n	$\mathcal{R}_n(h_{\ell r})$	$\log \mathcal{R}_n(h_{\ell r})/\mathcal{R}_{2n}(h_{\ell r}) /\log(2)$
.00	2	.206E-04	
.06	4	.309E-06	6.06
.05	8	.200E-09	10.60
.11	16	-.727E-11	4.78
		$\ell = 4, r = 4$	$2\xi + 1 = 8.02$
time	n	$\mathcal{R}_n(h_{\ell r})$	$\log \mathcal{R}_n(h_{\ell r})/\mathcal{R}_{2n}(h_{\ell r}) /\log(2)$
.00	2	.170E-06	
.06	4	.789E-08	4.42
.05	8	-.000E-00	

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