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COMPLEX ORTHOGONALITY ON THE SEMICIRCLE WITH RESPECT TO GEGENBAUER WEIGHT: THEORY AND APPLICATIONS

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Complex polynomials $\{\pi_k\}$, $\pi_k(z) = z^k + \cdots$, orthogonal with respect to a complex-valued inner product

$$(f, g) = \int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})d\theta, \quad w(z) = (1 - z^2)^{\lambda-\frac{1}{2}},\ \lambda > -\frac{1}{2},$$

are considered and used in construction of Gauss-Gegenbauer quadrature formulas over the semicircle. Some numerical results regarding error bounds for these formulas, applied to analytic functions, are given. Applications are discussed involving numerical differentiation and the computation of Cauchy principal value integrals with Gegenbauer weights.

1 Introductions to Orthogonal Polynomials

1.1 Types of Orthogonal Polynomials

Given a real linear space of functions X, an inner product (f, g) defined is a mapping of X^2 into $\mathbb{R}$ such that

(a) $(f + g, h) = (f, h) + (g, h)$	(Linearity),
(b) $(\alpha f, g) = \alpha(f, g)$	(Homogeneity),
(c) $(f, g) = (g, f)$	(Symmetry),
(d) $(f, f) > 0\,,\ (f, f) = 0 \Leftrightarrow f = 0$	(Positivity),

where $f, g, h \in X$ and α is a real scalar.

If X is a complex linear space of functions, then the inner product (f, g) maps X^2 into $\mathbb{C}$ and requirement (c) is replaced by

(c′) $(f, g) = \overline{(g, f)}$ (Hermitian Symmetry).

The bar in the above line designates the complex conjugate.

A system of polynomials $\{p_k\}$, where

(1.1.1) $$p_k(t) = t^k + \text{terms of lower degree},\ k = 0, 1, \ldots ,$$

and

$$(p_k, p_m) = 0 \ \ (k \neq m), \quad (p_k, p_m) > 0 \ \ (k = m)\,,$$

is called a system of (monic) orthogonal polynomials with respect to the inner product $(.\,,\,.)$.

The most common type of orthogonality is with respect to the following inner product

$$(f, g) = \int_{\mathbb{R}} f(t)g(t)d\lambda(t)\ , \tag{1.1.2}$$

where $d\lambda(t)$ is a nonnegative measure on the real line $\mathbb{R}$, with compact or infinite support, for which all moments $\mu_k = \int_{\mathbb{R}} t^k d\lambda(t),\ k = 0, 1, \ldots,$ exist and are finite, and $\mu_0 > 0$. Then the (monic) orthogonal polynomials $\{p_k\}$ satisfy the fundamental three-term recurrence relation

$$\begin{aligned} &p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ &p_{-1}(t) = 0, \quad p_0(t) = 1, \end{aligned} \tag{1.1.3}$$

where the coefficients a_k and b_k are given by

$$a_k = \frac{(tp_k, p_k)}{(p_k, p_k)}, \qquad k = 0, 1, 2, \ldots\ ,$$

$$b_k = \frac{(p_k, p_k)}{(p_{k-1}, p_{k-1})}, \qquad k = 1, 2, \ldots\ .$$

We note that $b_k > 0,\ k \geq 1$. The coefficient b_0 in (1.1.3) is arbitrary, but the definition $b_0 = \mu_0 = \int_{\mathbb{R}} d\lambda(t)$ is sometimes convenient.

The typical examples of these polynomials are classical orthogonal polynomials of Legendre, Chebyshev, Gegenbauer, Jacobi, Laguerre and Hermite.

The second type of orthogonality is orthogonality on the unit circle, with respect to the inner product

$$(f, g) = \int_0^{2\pi} f\left(e^{i\theta}\right) \overline{g\left(e^{i\theta}\right)} d\mu(\theta), \quad d\mu(\theta) \geq 0.$$

These polynomials have been introduced and studied by Szegö [29]. The monic orthogonal polynomials $\{\phi_k\}$ on the unit circle satisfy the recurrence relation (but not three-term relation like (1.1.3))

$$\phi_{k+1}(z) = z\phi_k(z) + \phi_k(0)z^k\overline{\phi}_k(1/z), \quad k = 0, 1, \ldots\ .$$

For details see Nevai [24]. Similarly, orthogonal polynomials on a rectifiable curve or arc lying in the complex plane can be considered (see for example, Refs. [14] & [30]). Also, complex orthogonal polynomials may be constructed with double integrals. Namely, introducing the inner product by

$$(f, g) = \iint_B f(z)\overline{g(z)}w(z)dxdy$$

for a suitable positive weight functions $w(z)$, where B is a bounded region lying in the complex plane, a system of orthogonal polynomials can be generated (see Carlemann [3] and Bochner [11]).

Recently, one new type of orthogonality – orthogonality on the semicircle – has been introduced by Gautschi and Milovanović [10] (see also Ref. [9]). The inner product is given by

$$(f,g)=\int_\Gamma f(z)g(z)(iz)^{-1}dz\,, \tag{1.1.4}$$

where Γ is the semicircle $\Gamma=\left\{z\in\mathbb{C}:z=e^{i\theta},\ 0\le\theta\le\pi\right\}$. Alternatively,

$$(f,g)=\int_0^\pi f\left(e^{i\theta}\right)g\left(e^{i\theta}\right)d\theta\,. \tag{1.1.5}$$

Note that this inner product does not satisfy the conditions (c′) and (d). Namely, the second factor in (1.1.4), i.e. (1.1.5), is not conjugated, so that this product has no Hermitian Symmetry, but is possesses the standard Symmetry property (c).

The corresponding (monic) orthogonal polynomials exist uniquely and satisfy a three-term recurrence relation like (1.1.3), because of the property $(zf,g)=(f,zg)$.

Later, Gautschi, Landau and Milovanović [11] have considered complex polynomials orthogonal with respect to a complex-valued inner product

$$\begin{aligned}(f,g)=&\int_\Gamma f(z)g(z)w(z)(iz)^{-1}dz\\ =&\int_0^\pi f\left(e^{i\theta}\right)g\left(e^{i\theta}\right)w\left(e^{i\theta}\right)d\theta\,,\end{aligned} \tag{1.1.6}$$

under suitable assumptions on the "weight function" w.

Let $w:(-1,1)\mapsto\mathbb{R}_+$ be a weight function, which can be extended to a function $w(z)$ holomorphic in the half disc $D_+=\{z\in\mathbb{C}:|z|<1,\ \operatorname{Im}z>1\}$. Under the assumption

$$\operatorname{Re}(1,1)=\operatorname{Re}\int_0^\pi w\left(e^{i\theta}\right)d\theta\ne0\,, \tag{1.1.7}$$

the monic, complex polynomials $\{\pi_k\}$ orthogonal with respect to the inner product (1.1.6) satisfy the recurrence relation

$$\begin{aligned}&\pi_{k+1}(z)=(z-i\alpha_k)\pi_k(z)-\beta_k\pi_{k-1}(z)\,,\quad k=0,1,2,\dots\,,\\ &\pi_{-1}(z)=0\,,\ \pi_0(z)=1\,,\end{aligned} \tag{1.1.8}$$

where coefficients α_k and β_k are given by

$$\begin{aligned}&\alpha_0=\theta_0-ia_0\,,\quad \alpha_k=\theta_k-\theta_{k-1}-ia_k\,,\quad k\ge1\,,\\ &\beta_k=\theta_{k-1}(\theta_{k-1}-ia_{k-1})\,,\quad k\ge1\,,\\ &\theta_{-1}=\mu_0=(1,1)\,,\quad \theta_k=ia_k+\frac{b_k}{\theta_{k-1}}\,,\quad k\ge0\,,\end{aligned}$$

and a_k, b_k are the recursion coefficients in the relation (1.1.3) for (real) polynomials orthogonal with respect to (1.1.2), where $d\lambda(t) = w(t)dt$ on $(-1, 1)$.

Several interesting properties of such polynomials $\{\pi_k\}$ were shown in Ref. [11], especially for Gegenbauer weight. In this paper we consider only polynomials orthogonal with respect to the Gegenbauer weight. In Chapter 2 we construct Gauss-Christoffel quadrature formulae with Gegenbauer weight for integration over the semicircle and give some results regarding error bounds for such formulas, applied to analytic functions. In Chapter 3 we apply obtained quadratures to numerical differentiation of analytic functions and to compute the Cauchy principal value of integrals with Gegenbauer weight.

1.2 Orthogonal Polynomials on the Semicircle with Respect to Gegenbauer Weight

In this section and further we use the Gegenbauer weight

$$w(z) = (1 - z^2)^{\lambda - \frac{1}{2}}, \quad \lambda > -\frac{1}{2}\,. \tag{1.2.1}$$

The assumption (1.1.7) is satisfied. Namely, $\mu_0 = (1, 1) = \pi$. The corresponding polynomials $\{\pi_k\}$ orthogonal on the semicircle can be expressed in terms of monic Gegenbauer polynomials $\widehat{C}_k(z)$ (Ref. [11])

$$\pi_n(z) = \widehat{C}_n^\lambda(z) - i\theta_{n-1}\widehat{C}_{n-1}^\lambda(z)\,,$$

where θ_{n-1} is given recursively by

$$\theta_0 = \frac{\Gamma\left(\lambda + \frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\lambda + 1)}\,, \quad \theta_n = \frac{n(n + 2\lambda - 1)}{4(n + \lambda)(n + \lambda - 1)} \cdot \frac{1}{\theta_{n-1}}\,, \quad n = 1, 2, \ldots\,.$$

Alternatively,

$$\theta_n = \frac{1}{\lambda + n} \cdot \frac{\Gamma\left(\frac{n+2}{2}\right)\Gamma\left(\lambda + \frac{n+1}{2}\right)}{\Gamma\left(\frac{n+1}{2}\right)\Gamma\left(\lambda + \frac{n}{2}\right)}\,, \quad n \geq 1\,. \tag{1.2.2}$$

In the special cases we have:

(1) For $\lambda = 0$ (Chebyshev case): $\theta_0 = 1\,,\ \theta_n = \dfrac{1}{2}\,,\ n \geq 1\,,$

(2) For $\lambda = \dfrac{1}{2}$ (Legendre case): $\theta_n = \dfrac{2}{2n+1}\left(\dfrac{\Gamma((n+2)/2)}{\Gamma((n+1)/2)}\right)^2\,,$

(3) For $\lambda = 1$ (Chebyshev case of the second kind): $\theta_n = \dfrac{1}{2}\,,\ n \geq 0\,.$

The polynomials $\{\pi_k\}$ satisfy the three-term recurrence relation (1.1.8), where

$$\alpha_0 = \theta_0\,, \quad \alpha_k = \theta_k - \theta_{k-1}\,, \quad \beta_k = \theta_{k-1}^2\,, \quad k \geq 1\,.$$

Using Stirling's formula in (1.2.2), we find that $\theta_n \to \dfrac{1}{2}\,,\ \alpha_n \to 0\,,\ \beta_n \to \dfrac{1}{4}\,,$ when $n \to +\infty$.

The norm of π_n is given by

$$||\pi_n|| = \sqrt{\pi}(\theta_0\,\theta_1\,\cdots\,\theta_{n-1}) = \frac{\Gamma\left(\dfrac{n+1}{2}\right)\Gamma\left(\lambda+\dfrac{n}{2}\right)}{\Gamma(\lambda+n)}\,. \tag{1.2.3}$$

The functions

$$\rho_k(z) = \int_\Gamma \frac{\pi_k(\zeta)}{z-\zeta}\cdot\frac{w(\zeta)}{i\zeta}\,d\zeta\,, \tag{1.2.4}$$

where

$$\Gamma = \left\{\zeta \in \mathbb{C} : \zeta = e^{i\theta},\ 0 \leq \theta \leq \pi\right\}\,,$$

are called the functions of the second kind. It is easily seen that they also satisfy the same recurrence relations as $\{\pi_k\}$. Indeed, from (1.1.8), for $z = \zeta$, multiplying by $w(\zeta)(i\zeta)^{-1}/(z-\zeta)$ and integrating, we obtain

$$\rho_{k+1}(z) = (z - i\alpha_k)\rho_k(z) - \int_\Gamma \pi_k(\zeta)\,\frac{w(\zeta)}{i\zeta}\,d\zeta - \beta_k\rho_{k-1}(z)\,.$$

By orthogonality, the integral on the right side of the above equality vanishes if $k \geq 1$, and equals $\mu_0(=\pi)$ if $k = 0$. If we define $\rho_{-1}(z) = 1$ (and $\beta_0 = \mu_0 = \pi$), we have

$$\rho_{k+1}(z) = (z - i\alpha_k)\rho_k(z) - \beta_k\rho_{k-1}(z)\,, \quad k = 0, 1, 2, \ldots\,. \tag{1.2.5}$$

On analytic and numerical computations of the functions ρ_k corresponding to Jacobi orthogonal polynomials on $(-1, 1)$, there is a very interesting paper of Gautschi and Wimp [13].

The following theorem gives and asymptotic form of ρ_k.

Theorem 1.2.1. *For $|z|$ sufficiently large, we have*

$$\rho_n(z) = \frac{||\pi_n||^2}{z^{n+1}}\left(1 + O\Big(\frac{1}{2}\Big)\right)\,, \tag{1.2.6}$$

where the norm $||\pi_n||$ is given by (1.2.3).

Proof. Let $\zeta \in \Gamma = \left\{\zeta \in \mathbb{C} : \zeta = e^{i\theta},\ 0 \leq \theta \leq \pi\right\}$ and $z \in \mathbb{C}$, such that $|z| > 1$. Since

$$\frac{1}{z-\zeta} = \frac{1}{z}\cdot\frac{1}{1-\dfrac{\zeta}{z}} = \sum_{k=0}^{n}\left(\frac{\zeta}{z}\right)^k + \frac{\zeta^{n+1}}{(z-\zeta)z^{n+1}} \quad (n \in \mathbb{N})\,,$$

we have

$$\rho_n(z) = \sum_{k=0}^{n} \frac{1}{z^{k+1}} \int_\Gamma \zeta^k \pi_n(\zeta) \frac{w(\zeta)}{i\zeta} \, d\zeta + \frac{1}{z^{n+1}} r_n(z) \,,$$

where

$$r_n(z) = \int_\Gamma \frac{\zeta^{n+1}\pi_n(\zeta)}{z-\zeta} \cdot \frac{w(\zeta)}{i\zeta} \, d\zeta \,.$$

For $|z|$ sufficiently large, there exists a constant $C > 0$ such that $|r_n(z)| < \dfrac{C}{|z|}$ and $r_n(z) \to 0$, when $|z| \to \infty$.

Because of orthogonality $\big(\zeta^k, \pi_n(\zeta)\big) = 0$, $k < n$, we obtain

$$\rho_n(z) = \frac{||\pi_n||^2}{z^{n+1}} + \frac{1}{z^{n+1}} r_n(z) \,,$$

i.e. (1.2.6).

The quantities $\dfrac{\rho_n(z)}{\pi_n(z)}$, $|z| > 1$, are important in getting error bounds for Gaussian quadrature formulas over semicircle, applied to analytic functions.

Introduced the polynomials

$$q_k(z) = \int_\Gamma \frac{\pi_k(z) - \pi_k(\zeta)}{z-\zeta} \cdot \frac{w(\zeta)}{i\zeta} \, d\zeta \,,$$

which are called the polynomials associated with the orthogonal polynomials π_k, we see that

$$\rho_k(z) = \pi_k(z)\rho_0(z) - q_k(z) \,.$$

The polynomials $\{q_k\}$ satisfy the same three-term recurrence relation

$$\begin{aligned} q_{k+1}(z) &= (z - i\alpha_k)q_k(z) - \beta_k q_{k-1}(z) \,, \quad k = 1, 2, \ldots \,, \\ q_0(z) &= 0 \,, \quad q_1(z) = \mu_0 = \pi \,. \end{aligned} \tag{1.2.7}$$

If we define $q_{-1}(z) = -1$ and $\beta_0 = \mu_0 = \pi$, we can note that (1.2.7) also holds for $k = 0$ (see Ref. [8]).

Using the recurrence relations for $\{\pi_k\}$, $\{\rho_k\}$ and $\{q_k\}$ ((1.1.8), (1.2.5) and (1.2.7), respectively), where

(a) $\pi_{-1}(z) = 0$, $\quad \pi_0(z) = 1$;

(b) $\rho_{-1}(z) = 1$, $\quad \rho_0(z) = F(z) = \displaystyle\int_\Gamma (z-\zeta)^{-1} w(\zeta)(i\zeta)^{-1} \, d\zeta$;

(c) $q_{-1}(z) = -1$, $\quad q_0(z) = 0$,

it is easily proved the following identity of Christoffel-Darboux type:

THEOREM 1.2.2. *Let $\{f_k\}$ and $\{g_k\}$ satisfy the three-term recurrence relation of the form* (1.1.8) *and*

$$S_k(z, w) = f_{k+1}(z)g_k(w) - g_{k+1}(w)f_k(z) \,.$$

Then the identity

$$(z-w)\sum_{k=0}^{n}\frac{f_k(z)g_k(z)}{\beta_0\,\beta_1\,\ldots\,\beta_k}=\frac{S_n(z,w)}{\beta_0\,\beta_1\,\ldots\,\beta_n}-S_{-1}(z,w)$$

holds, where β_k are the recursion coefficient in (1.1.8). *In special cases we have:*

$$\begin{array}{llll}
\text{(a)} & f_k:=\pi_k\,, & g_k=\pi_k\,, & S_{-1}(z,w)=0\,;\\
\text{(b)} & f_k:=\pi_k\,, & g_k=\rho_k\,, & S_{-1}(z,w)=1\,;\\
\text{(c)} & f_k:=\pi_k\,, & g_k=q_k\,, & S_{-1}(z,w)=-1\,;\\
\text{(d)} & f_k:=\rho_k\,, & g_k=\rho_k\,, & S_{-1}(z,w)=F(z)-F(w)\,;\\
\text{(e)} & f_k:=\rho_k\,, & g_k=q_k\,, & S_{-1}(z,w)=-1\,;\\
\text{(f)} & f_k:=q_k\,, & g_k=q_k\,, & S_{-1}(z,w)=0\,.
\end{array}$$

An interesting property of the polynomials $\{\pi_k\}$ is a distribution of zeros. It was shown (Theorem 6.5 and 6.7 in Ref. [11]) that all zeros of $\pi_k(z)\,,\ k\geq 2\,,$ are simple and contained in the upper unit half disc

$$D_+=\{z\in\mathbb{C}:\ |z|<1\,,\ \operatorname{Im} z>0\}\,.$$

2 Gauss-Gegenbauer Quadrature over the Semicircle

2.1 Construction of the Formulae

In this section we will construct a Gauss-Christoffel quadrature formula over the semicircle

$$\int_0^{\pi} f\left(e^{i\theta}\right)w\left(e^{i\theta}\right)\,d\theta=\sum_{\nu=1}^{n}\sigma_\nu f(\zeta_\nu)+R_n(f)\,, \tag{2.1.1}$$

which is exact for all algebraic polynomials of degree at most $2n-1$, i.e. $R_n(\mathbb{P}_{2n-1})=0$. The weight function is given by (1.2.1). The nodes $\zeta_\nu=\zeta_\nu^{(n)}$ are precisely the zeros of $\pi_n(z)$. By the same procedure as in Ref. [10] (see also Ref. [15]), we can determine the weights $\sigma_\nu=\sigma_\nu^{(n)}$. Because of that, we will consider an eigenvalue problem for Jacobi matrix

$$J_n=\begin{bmatrix} i\alpha_0 & \theta_0 & & & \mathrm{O}\\ \theta_0 & i\alpha_1 & \theta_1 & & \\ & \theta_1 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2}\\ \mathrm{O} & & & \theta_{n-2} & i\alpha_{n-1}\end{bmatrix}.$$

Namely, using the corresponding recurrence relation for the orthogonal polynomials π_n^* $(\pi_k^*(z) = \pi_k(z)/||\pi_k||\,,\ ||\pi_k||^2 = \pi(\beta_1\,\beta_2\,\ldots\,\beta_k) = \pi(\theta_0\,\theta_1\,\ldots\,\theta_{k-1})^2\,,$ $||\pi_0||^2 = \pi)$

$$\begin{aligned}&\theta_k\pi_{k+1}^* = (z - i\alpha_k)\pi_k^*(z) - \theta_{k-1}\pi_{k-1}^*(z)\,,\quad k = 0,1,\ldots\,,\\&\pi_{-1}^*(z) = 0\,,\quad \pi_0^*(z) = 1/\sqrt{\pi}\,,\end{aligned}$$

and putting $k = 0,1,\ldots,n-1$, we obtain the following system of linear equations

$$z\mathbf{q}^*(z) = J_n\mathbf{q}^*(z) + \theta_{n-1}\pi_n^*(z)\mathbf{e}_n\,,$$

where

$$\begin{aligned}&\mathbf{q}^*(z) = [\pi_0^*(z)\,,\,\pi_1^*(z)\,,\,\ldots\,,\,\pi_{n-1}^*(z)]^T\,,\\&\mathbf{e}_n = [0,\,0\,\ldots,\,1]^T\,.\end{aligned}$$

Thus, $\pi_n^*(\zeta_\nu) = 0$ if and only if $\zeta_\nu\mathbf{q}^*(\zeta_\nu) = J_n\mathbf{q}^*(\zeta_\nu)$, where ζ_ν is an eigenvalue of the Jacobi matrix J_n, and $\mathbf{q}^*(\zeta_\nu)$, is the corresponding eigenvector. By a similarity transformation with diagonal matrix

$$D_n = \operatorname{diag}(1\,,\,i\theta_0\,,\,i^2\theta_0\theta_1\,,\,i^3\theta_0\theta_1\theta_2\,,\,\ldots) \in \mathbb{C}^{n\times n}\,,$$

the complex Jacobi matrix J_n can be transformed to the real nonsymmetric tridiagonal matrix

$$A_n = -iD_n^{-1}J_nD_n = \begin{bmatrix} \alpha_0 & \theta_0 & & & \mathrm{O}\\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2}\\ \mathrm{O} & & & -\theta_{n-2} & \alpha_{n-1}\end{bmatrix},$$

whose eigenvalues are $\eta_\nu = -i\zeta_\nu$. Defining

$$\mathbf{p}(z) = D_n^{-1}\mathbf{q}^*(z)\,,$$

the new eigenvalue problem is

$$A_n\mathbf{p}(\zeta_\nu) = \eta_\nu\mathbf{p}(\zeta_\nu)\,,$$

where $\mathbf{p}(\zeta_\nu)$ is an eigenvector of the real matrix A_n corresponding to the eigenvalue $\eta_\nu = -i\zeta_\nu$. Denote by V_n the matrix of the eigenvectors of the matrix A_n, each normalized so that the first component is equal to 1. Then

$$V_n = [\mathbf{v}_1\,,\,\mathbf{v}_2\,,\,\ldots\,,\,\mathbf{v}_n]\,,\quad \mathbf{v}_\nu = \sqrt{\pi}\,\mathbf{p}(\zeta_\nu)\,.$$

Substituting in (2.1.1) $f(z) = \pi_k^*(z)$, $k = 0,1,\ldots,n-1$, we obtain

$$\sum_{\nu=1}^{n}\sigma_\nu\pi_k^*(\zeta_\nu) = \frac{\mu_0}{\sqrt{\pi}}\,\delta_{k0}\,,\quad k = 0,1,\ldots,n-1\,,$$

where $\mu_0 = \int_0^\pi w(e^{i\theta})\,d\theta = \pi w(0) = \pi$ and δ_{k0} is Kronecker's delta. Putting $\sigma = [\sigma_1\,,\,\sigma_2\,,\,\ldots\,,\,\sigma_n]^T$, this system of linear equations can be represented in the form

$$V_n\sigma = \pi\mathbf{e}_1\,,$$

where $\mathbf{e}_1 = [1, 0, \ldots, 0]^T$ (the first coordinate vector).

Using the EISPACK routine HQR2 in Ref. [27], pp. 248 we determine the matrix V_n and η_ν, i.e. $\zeta_\nu\,,\ \nu = 1, \ldots, n\,,$ and then using the LINPACK routine CGECO and CGESL in Ref. [6], Chap. 1 we find the weights $\sigma_\nu,\ \nu = 1, \ldots, n\,.$

In Table 2.1.1 we give the parameters of Gauss-Christoffel formulae, with Chebyshev weight $w(z) = (1 - z^2)^{-1/2}$, for $n = 2,\,3,\,5,\,10$ and $20\,$. Similarly, in Table 2.1.2 we give the corresponding parameters for the weight $w(z) = (1 - z^2)^{1/2}\,$. The Legendre case ($\lambda = 1/2$) was consider in Ref. [10]. Notice that σ_ν is real if ζ_ν is purely imaginary and $\sigma_{\nu+1} = \overline{\sigma}_\nu$ if $\zeta_{\nu+1} = -\overline{\zeta}_\nu\,$. All the parameters are given with 10 decimals.

Table 2.1.1: Gauss-Gegenbauer formula for $\lambda = 0$ and $n = 2,\,3,\,5,\,10,\,20$

n	ν	ζ_ν	σ_ν
2	$1,2$	$\pm 0.6614378278 + i0.25$	$1.5707963268 \pm i1.7811156176$
3	$1,2$	$\pm 0.8330737868 + i0.0711936904$	$0.4439951945 \pm i1.3638988336$
	3	$i0.3576126192$	2.2536022646
5	$1,2$	$\pm 0.9419742963 + i0.0131804455$	$0.0961180099 \pm i0.7284541059$
	$3,4$	$\pm 0.5293892203 + i0.1170312173$	$0.4793033286 \pm i1.1121917500$
	5	$i0.2395766744$	1.9907499765
10	$1,2$	$\pm 0.9864752305 + i0.0014308303$	$0.0183166848 \pm i0.3342240223$
	$3,4$	$\pm 0.8805690003 + i0.0128801054$	$0.0277856841 \pm i0.3734785990$
	$5,6$	$\pm 0.6808918333 + i0.0360385425$	$0.0621933439 \pm i0.4775784585$
	$7,8$	$\pm 0.1253750607 + i0.1266268186$	$1.2388003990 \pm i0.8664290060$
	$9,10$	$\pm 0.4122690798 + i0.0730237032$	$0.2237002150 \pm i0.7339498999$
20	$1,2$	$\pm 0.9967637119 + i0.0001661622$	$0.0041819658 \pm i0.1615221229$
	$3,4$	$\pm 0.9710003056 + i0.0014954851$	$0.0046333112 \pm i0.1657894264$
	$5,6$	$\pm 0.9201470767 + i0.0041557982$	$0.0056638997 \pm i0.1749052444$
	$7,8$	$\pm 0.8455362249 + i0.0081585184$	$0.0076044577 \pm i0.1902346507$
	$9,10$	$\pm 0.7491309976 + i0.0135448966$	$0.0112187149 \pm i0.2144721022$
	$11,12$	$\pm 0.6334930531 + i0.0204297239$	$0.0183978016 \pm i0.2529778571$
	$13,14$	$\pm 0.0631322988 + i0.0768826489$	$1.1393772591 \pm i0.7016087342$
	$15,16$	$\pm 0.2071163626 + i0.0557871654$	$0.2648753570 \pm i0.6737226970$
	$17,18$	$\pm 0.3578140193 + i0.0402782196$	$0.0802264387 \pm i0.4354744109$
	$19,20$	$\pm 0.5017700872 + i0.0291013815$	$0.0346171211 \pm i0.3173012802$

Example 2.1.1. $w(z) = (1 - z^2)^{\lambda - 1/2},\ \lambda > -1/2\,,\ c > 0\,,$

$$I_\lambda(c) = \int_0^\pi w\left(e^{i\theta}\right)\exp\left(ce^{i\theta}\right)\,d\theta = \pi + i\int_{-1}^{1} w(x)\frac{\sinh(cx)}{x}\,dx\,.$$

Table 2.1.2: Gauss-Gegenbauer formula for $\lambda = 1$ and $n = 2,\ 3,\ 5,\ 10,\ 20$

n	ν	ζ_ν	σ_ν
2	$1,2$	$\pm 0.4330127019 + i0.25$	$1.5707963268 \pm i0.9068996821$
3	$1,2$	$\pm 0.6535706393 + i0.1075399273$	$0.4364859430 \pm i0.6353875041$
	3	$i0.2849201455$	2.2686207675
5	$1,2$	$\pm 0.8456395748 + i0.0290906887$	$0.0594249834 \pm i0.1845742718$
	$3,4$	$\pm 0.4427783801 + i0.1168384260$	$0.5149777883 \pm i0.8131061591$
	5	$i0.2081417706$	1.9927871103
10	$1,2$	$\pm 0.9558839022 + i0.0042428564$	$0.0039928133 \pm i0.0267971996$
	$3,4$	$\pm 0.8275965485 + i0.0169982154$	$0.0189583100 \pm i0.1125358905$
	$5,6$	$\pm 0.6271990214 + i0.0386782128$	$0.0618881850 \pm i0.2815813023$
	$7,8$	$\pm 0.1140015897 + i0.1185009012$	$1.2484307106 \pm i0.8080856375$
	$9,10$	$\pm 0.3754517574 + i0.0715798141$	$0.2375263079 \pm i0.6132428252$
20	$1,2$	$\pm 0.9883014969 + i0.0005721194$	$0.0002662835 \pm i0.0036001003$
	$3,4$	$\pm 0.9534824217 + i0.0022887369$	$0.0011093098 \pm i0.0145750841$
	$5,6$	$\pm 0.8963663489 + i0.0051533125$	$0.0026841237 \pm i0.0335156272$
	$7,8$	$\pm 0.8183074519 + i0.0091816674$	$0.0053441082 \pm i0.0616670850$
	$9,10$	$\pm 0.7211656456 + i0.0144218674$	$0.0098826185 \pm i0.1014958341$
	$11,12$	$\pm 0.6072806483 + i0.0209961264$	$0.0182462928 \pm i0.1580346653$
	$13,14$	$\pm 0.0601777665 + i0.0741386587$	$1.1410946350 \pm i0.6830593808$
	$15,16$	$\pm 0.1972558833 + i0.0543276979$	$0.2721901872 \pm i0.6403439177$
	$17,18$	$\pm 0.3411506891 + i0.0397239575$	$0.0839407402 \pm i0.3818629864$
	$19,20$	$\pm 0.4794691593 + i0.0291958559$	$0.0360380280 \pm i0.2423879159$

The case $\lambda = 1/2$ was considered in Ref. [10]. Here, we consider the Chebyshev case $(\lambda = 0)$. The true values of the integral $\operatorname{Im} I_0(c)$ (to 40 decimals) are listed in Table 2.1.3, for $c = 0.2,\ 0.6,\ 1.,\ 2.,\ 6.,\ 10.$ and 20. These results were obtained by Gauss-Chebyshev formulas on $(-1, 1)$ in MP aritmetic [2].

Now, we apply the Gauss-Gegenbauer rule (2.1.1) with $f(z) = \exp(cz)$. Table 2.1.4 shows the corresponding relative errors in the real and imaginary parts of $I_0(c)$, for $n = 2(1)5$ and $c = 0.2,\ 0{,}6$ and 1.0. For larger value of $c\,(c = 2.0,\ 6.0,\ 10.0$ and $20.0)$ and $n = 5,\ 8,\ 12,\ 16$ and 20, the corresponding results are presented in Table 2.1.5. In the empty entries of this table the errors are close to machine precision ($\cong 8.882 \times 10^{-16}$ in double precision on the PC ZENITH).

2.2 Error Bounds for Quadrature of Analytic Functions

Following Gautschi and Varga [12] we can give error bounds for the Gauss-Gegenbauer quadratures (2.1.1), applied to analytic functions, using contour integral representation of the remainder term. We assume that f is analytic and

Table 2.1.3: True values of the imaginary part of the integral $I_\lambda(c)$

c	$\operatorname{Im} I_\lambda(c)$
0.2	0.6304160699 0754536678 8880643322 2922467067
0.6	1.9422731437 6744951192 7710675910 5302535350
1.0	3.4134066963 7963272959 3628381683 1800902060
2.0	8.7179255997 9107946874 3577972570 2815852715
6.0	238.9068734682 0181695351 9847754042 4768871867
10.0	9402.9267475634 6627931909 0486926835 8572968343
20.0	140613285.5327413013 9382043732 7261787938 9495862996

Table 2.1.4: Relative errors in real and imaginary parts

n	$c = 0.2$		$c = 0.6$		$c = 1.0$	
2	1.67(−5)	3.33(−6)	1.36(−3)	2.65(−4)	1.07(−2)	1.98(−3)
3	5.56(−9)	7.92(−10)	4.08(−6)	5.66(−7)	8.88(−5)	1.17(−5)
4	9.93(−13)	1.10(−13)	6.55(−9)	7.07(−10)	3.95(−7)	4.04(−8)
5	4.58(−16)	7.04(−16)	6.55(−12)	5.78(−13)	1.09(−9)	9.17(−11)

regular in a certain domain G which contains the upper unit half disc

$$D_+ = \Big\{ z \in \mathbb{C} : |z| < 1\,,\ \operatorname{Im} z > 0 \Big\}$$

in its interior. Using Cauchy's integral representation of the function

$$f(\zeta) = \frac{1}{2\pi i} \int_C \frac{f(z)}{z - \zeta}\, d\zeta\,,$$

where C is a contour in G surrounding D_+, the remainder term $R_n(f)$ in (2.1.1) can be represented in the form

$$R_n(f) = \frac{1}{2\pi i} \int_C K_n(z) f(z)\, dz\,, \tag{2.2.1}$$

Table 2.1.5: Relative errors in real and imaginary parts

n	$c = 2.0$		$c = 6.0$		$c = 10.0$		$c = 20.0$	
5	1.2(−6)	7.8(−8)	1.2(−1)	8.7(−4)	5.6(1)	1.8(−2)	4.7(6)	2.1(−1)
8	2.0(−13)	8.8(−15)	1.3(−5)	6.0(−8)	9.7(−2)	1.9(−5)	1.8(5)	4.9(−3)
12			2.5(−12)	6.9(−15)	9.2(−7)	1.2(−10)	1.9(2)	3.4(−6)
16					3.1(−12)	1.5(−14)	2.2(−2)	3.0(−10)
20							3.8(−7)	1.0(−14)

where the kernel K_n is given by

$$K_n(z) = R_n\left(\frac{1}{z-\cdot}\right) = \int_\Gamma \frac{1}{z-\zeta}\cdot\frac{w(\zeta)}{i\zeta}\,d\zeta - \sum_{\nu=1}^{n}\frac{\sigma_\nu}{z-\zeta_\nu}\,. \tag{2.2.2}$$

Using the orthogonal polynomials on the semicircle $\pi_n(z)$ and their associated polynomials $q_n(z)$, we find that

$$\frac{q_n(z)}{\pi_n(z)} = \sum_{\nu=1}^{n}\frac{\sigma_\nu}{z-\zeta_\nu}\,,$$

where the Christoffel numbers are given by

$$\sigma_\nu = \frac{q_n(\zeta_\nu)}{\pi_n'(\zeta_\nu)} = \frac{1}{\pi_n'(\zeta_\nu)}\int_\Gamma \frac{\pi_n(\zeta)}{z-\zeta}\cdot\frac{w(\zeta)}{i\zeta}\,d\zeta\,,\quad \nu=1,\ldots,n\,.$$

Then we have

$$K_n(z) = \frac{1}{\pi_n(z)}\int_\Gamma \frac{\pi_n(\zeta)}{z-\zeta}\cdot\frac{w(\zeta)}{i\zeta}\,d\zeta = \frac{\rho_n(z)}{\pi_n(z)}\,. \tag{2.2.3}$$

On the other hand, the kernel $K_n(z)$ can be expressed in the form

$$K_n(z) = \sum_{k=2n}^{\infty}\frac{R_n\left(\zeta^k\right)}{z^{k+1}}\qquad (|z|>1)\,. \tag{2.2.4}$$

Indeed, by expanding $(z-\zeta)^{-1}$ in powers of $\zeta/z,\ (|z|>1)$, one obtained from (2.2.2), that

$$K_n(z) = \sum_{k=0}^{\infty}\frac{R_n\left(\zeta^k\right)}{z^{k+1}}\,,$$

i.e. (2.2.4), because $R_n\left(\zeta^k\right)=0$ for $k=0,\,1,\,\ldots,\,2n-1$.

In order to find the first term in expansion (2.2.4) we will start from

$$\pi_n(z)^2 = z^{2n}+q(z)\,,$$

where $q\in\mathbb{P}_{2n-1}$. Then we have

$$||\pi_n||^2 = \int_0^\pi e^{i2n\theta}w(e^{i\theta})\,d\theta + \int_0^\pi q(e^{i\theta})w(e^{i\theta})\,d\theta\,,$$

i.e.,

$$||\pi_n||^2 = \sum_{\nu=1}^{n}\sigma_\nu q(\zeta_\nu) = -\sum_{\nu=1}^{n}\sigma_\nu\zeta_\nu^{2n} = R_n(\zeta^{2n})\,,$$

because $0=\pi_n(\zeta_\nu)^2=\zeta_\nu^{2n}+q(\zeta_\nu)\,,\ \nu=1,\ldots,n$. Hence,

$$R_n(\zeta^{2n}) = ||\pi_n||^2 = \pi(\theta_0\,\theta_1\,\ldots\,\theta_{n-1})^2\,,$$

i.e.,

$$R_n(\zeta^{2n}) = \left(\frac{\Gamma\left(\dfrac{n+1}{2}\right)\Gamma\left(\lambda+\dfrac{n}{2}\right)}{\Gamma(\lambda+n)} \right)^2 . \tag{2.2.5}$$

So, the first term in (2.2.4) is $\dfrac{R_n(\zeta^{2n})}{z^{2n+1}}$.

If $\ell(C)$ denotes the lenght of the contour C, an estimate of the error R_n in (2.2.1) can be given by (see, for example, Refs. [4], [12] & [28])

$$|R_n(f)| \le \frac{\ell(C)}{2\pi} \max_{z\in C} |K_n(z)| \cdot ||f|| ,$$

where $||f|| = \max_{z\in C} |f(z)|$.

If we take the circle $C_r = \{z \in \mathbb{C} : |z| = r > 1\}$ as C, the last estimate becomes

$$|R_n(f)| \le rK_{n0}(r)||f|| , \tag{2.2.6}$$

where

$$K_{n0}(r) = \max_{z\in C_r} \left|K_n\left(re^{i\Psi}\right)\right| = \left|K_n\left(re^{i\Psi_0}\right)\right| . \tag{2.2.7}$$

Lemma 2.2.1. *There holds* $\overline{K_n(-\overline{z})} = -K_n(z)$.

Proof. Since $\pi_n(z) = \widehat{C}_n^\lambda(z) - i\theta_{n-1}\widehat{C}_{n-1}^\lambda(z)$ we conclude that

$$\pi_n(-\overline{z}) = (-1)^n\overline{\pi}_n(\overline{z}) = (-1)^n\overline{\pi_n(z)} .$$

Then

$$\begin{aligned} K_n(-\overline{z}) &= \frac{1}{\pi_n(-\overline{z})}\int_0^\pi w(e^{i\theta})\,\frac{\pi_n(e^{i\theta})}{-\overline{z}-e^{i\theta}}\,d\theta \\ &= \frac{1}{\pi_n(-\overline{z})}\int_0^\pi w(-e^{-i\theta})\,\frac{\pi_n(-e^{-i\theta})}{-\overline{z}+e^{-i\theta}}\,d\theta \qquad (\theta := \pi-\theta) \\ &= \frac{-1}{\overline{\pi_n(z)}}\int_0^\pi w(e^{-i\theta})\,\frac{\overline{\pi_n(e^{i\theta})}}{\overline{z}-e^{-i\theta}}\,d\theta , \end{aligned}$$

i.e.,

$$\overline{K_n(-\overline{z})} = -\frac{1}{\pi_n(z)}\int_0^\pi w(e^{i\theta})\frac{\pi_n(e^{i\theta})}{z-e^{i\theta}}\,d\theta = -K_n(z) .$$

In order to find the maximum of $\left|K_n\left(re^{i\Psi}\right)\right|$ on C_r, we will consider only the case when $|\Psi| \le \pi/2$ (because of Lemma 2.2.1). Moreover, numerical experiments show that $|K_n(z)| \ge |K_n(\overline{z})|$, when $\operatorname{Im} z > 0$. (It is interesting

Table 2.2.1: Numerical values of Ψ_0 for $\lambda = 0$

n	$r = 1.1$	$r = 1.5$	$r = 2.$	$r = 5.$
2	3.39494(−2)	1.14602(−1)	3.48505(−1)	1.25274(0)
3	2.71880(−2)	1.19470(−1)	2.14948(−1)	7.75105(−1)
5	1.57077(−2)	7.22458(−2)	1.34337(−1)	4.54503(−1)
10	8.06596(−3)	3.85359(−2)	7.06245(−2)	2.30733(−1)
20	4.36120(−3)	2.00058(−2)	3.63420(−2)	1.17297(−1)

Table 2.2.2: Numerical values of $K_{n0}(r)$ for $\lambda = 0$

n	$r = 1.1$	$r = 1.5$	$r = 2.$	$r = 5.$
2	2.74(0)	2.23(−1)	3.84(−2)	2.92(−4)
3	1.27(0)	3.20(−2)	2.66(−3)	2.89(−6)
5	2.30(−1)	6.70(−4)	1.34(−5)	2.94(−10)
10	2.75(−3)	4.36(−8)	2.51(−11)	3.18(−20)
20	3.84(−7)	1.89(−16)	9.06(−23)	3.85(−40)

to prove!). Numerical values of Ψ_0 in (2.2.7) are given in Table 2.2.1, for $r = 1.1, 1.5, 2., 5.$; $n = 2, 3, 5, 10, 20$; $\lambda = 0$. The corresponding values of $K_{n0}(r)$ are represented in Table 2.2.2.

Similar results were obtained for $\lambda = 0.5$ and $\lambda = 1$. Numerical results show that $K_{n0}(r)$ decreases when λ increases. For example, $K_{10,0}(2.)$ takes the following values 2.51(−11), 1.14(−11), 5.43(−12), when $\lambda = 0, 0.5, 1$, respectively.

For numerical computation of $K_n(z)$ we use the formula (2.2.3). Since ρ_n is a minimal solution of the basic three-term recurrence relation, for its computation is very convenient Gautschi's algorithm [8].

Example 2.2.1. For the integral in Example 2.1.1 we have $f(z) = \exp(cz)$. Let $z \in C_r$, i.e. $z = r\exp(i\theta)$, $r > 1$, $0 \le \theta \le 2\pi$. Then

$$|f(z)| = e^{cr\cos\theta} \le e^{cr}, \quad z \in C_r .$$

According to (2.2.6), we get

$$|R_n(f)| \le B_n(r) = rK_{n0}(r)e^{cr}, \quad r > 1 . \tag{2.2.8}$$

The bound on the right of (2.2.8) may be optimized as a function of r. So we obtain the following problem

$$\min_{r>1}\left\{ re^{cr} \max_{z\in C_r} |K_n(z)| \right\} = B_n(r_{\mathrm{opt}}) .$$

Using the Fibonnaci minimizing procedure we find the optimal values r_{opt} of r and corresponding optimal bounds. They are shown in Table 2.2.3, together with the modulus of the actual errors, for some selected values of c and n. Close to machine precision (indicated in Table 2.2.3 as m.p.), the actual error may be larger than the bound (see Gautschi and Varga [12]).

Table 2.2.3: Optimal Values of r and $B_n(r)$ and Actual Errors (e_n)

n	c	r_{opt}	$B_n(r_{\text{opt}})$	e_n	c	r_{opt}	$B_n(r_{\text{opt}})$	e_n
2	0.2	20.2	2.8(−4)	5.2(−5)	1.0	4.16	2.0(−1)	3.4(−2)
3		30.2	1.1(−7)	1.7(−8)		6.09	1.9(−3)	2.8(−4)
5		50.1	2.8(−15)	9.9(−16)		10.1	2.9(−8)	3.5(−9)
8		80.1	6.1(−28)	m.p.		16.0	9.7(−17)	m.p.
2	2.0	2.28	4.0(0)	6.2(−1)	6.0	1.22	1.9(−3)	1.8(2)
5		5.11	3.2(−5)	3.8(−6)		1.96	4.4(0)	4.3(−1)
8		8.07	6.7(−12)	6.3(−13)		2.86	4.8(−4)	4.3(−5)
10		10.1	6.3(−17)	m.p.		3.49	3.3(−7)	2.7(−8)
12		12.0	2.7(−22)	m.p.		4.13	1.1(−10)	8.1(−12)
5	10.0	1.44	3.2(3)	2.4(2)	20.0	1.14	8.4(8)	3.3(7)
10		2.25	2.0(−2)	1.5(−3)		1.43	6.5(5)	3.5(4)
20		4.13	4.3(−18)	m.p.		2.24	3.0(−5)	1.9(−6)

3 Some Applications in Numerical Analysis

3.1 Numerical Differentiation

Numerical differentiation of analytic functions is analyzed in a few papers [19], [20], [21], [31], [32]. The corresponding differentiation formulas are obtained mostly in Cauchy's integral formula and by applying the trapezoidal rule.

In order to obtain the differentiation formulas, we will use our quadrature formula (2.1.1). Such formulas in Legendre case ($\lambda = 0$) were considered in Ref. [22].

Let f be an analytic function on some domain containing the point a and a circular neighborhood of a with radius $h/2$. Using the standard central difference operator δ_h, defined by

$$\delta_h f(a) = \frac{1}{h}\left(f\left(a+\frac{h}{2}\right) - f\left(a-\frac{h}{2}\right)\right),$$

$he^{i\theta}$ instead of h, and integrating over the semicircle, we can show that

$$f'(a) = \frac{1}{\pi}\int_0^\pi \delta_{he^{i\theta}}\, f(a) w\left(e^{i\theta}\right)\, d\theta\,,$$

i.e.

$$f'(a) = \frac{1}{\pi h}\int_0^\pi e^{-i\theta}\left(f\left(a+\frac{h}{2}e^{i\theta}\right) - f\left(a-\frac{h}{2}e^{i\theta}\right)\right) w\left(e^{i\theta}\right)\, d\theta\,,$$

where $w(z) = (1 - z^2)^{\lambda - 1/2}$, $\lambda > -1/2$. Applying (2.1.1) to the integral on the right yields

$$(3.1.1) \quad f'(a) \cong D_n^h f(a) = \frac{1}{\pi h} \sum_{\nu=1}^{n} \frac{\sigma_\nu}{\zeta_\nu} \left(f\Big(a + \frac{h}{2}\,\zeta_\nu\Big) - f\Big(a - \frac{h}{2}\,\zeta_\nu\Big) \right).$$

THEOREM 3.1.1. *The error of the differentiation formula* (3.1.1) *is given by*

$$(3.1.2) \quad R(f) = f'(a) - D_n^h f(a) = \frac{1}{\pi} \sum_{k=n}^{\infty} \frac{f^{(2k+1)}(a)}{(2k+1)!} R_n\left(z^{2k}\right) \left(\frac{h}{2}\right)^{2k},$$

where $R_n\left(z^{2k}\right)$ *is defined in* (2.1.1). *The dominant error term is*

$$(3.1.3) \quad \frac{1}{\pi(2n+1)!} \left(\frac{\Gamma\left(\frac{n+1}{2}\right)\Gamma\left(\lambda + \frac{n}{2}\right)}{2^n \Gamma(\lambda + n)} \right)^2 h^{2n} f^{(2n+1)}(a).$$

Proof. As in Ref. [22], we develop $f\left(a \pm \frac{h}{2}\,\zeta_\nu\right)$ in Taylor series at $z = a$ and substitute these expressions in $D_n^h f(a)$. So we prove (3.1.2). Using (2.2.5) we obtain (3.1.3).

For real-valued analytic functions the formula (3.1.1) may be simplified. Namely, when n is even, and $\operatorname{Re}\zeta_\nu > 0$ for $\nu = 1, 2, \ldots, n/2$, one finds

$$(3.1.4) \quad D_n^h f(a) = \frac{2}{\pi h} \sum_{\nu=1}^{n/2} \operatorname{Re}\left(\frac{\sigma_\nu}{\zeta_\nu} \left(f\Big(a + \frac{h}{2}\,\zeta_\nu\Big) - f\Big(a - \frac{h}{2}\,\zeta_\nu\Big) \right) \right).$$

Especially, it is interesting in the simplest case: $n = 2$. Then we have

$$\zeta_{1,2} = \frac{1}{2}\left(i\theta_1 \pm \sqrt{\theta_1(4\theta_0 - \theta_1)} \right) = \pm x + iy,$$
$$\sigma_{1,2} = \frac{\pi}{2}\left(1 \pm i\frac{\theta_0 - y}{x} \right),$$

where

$$\theta_0 = \frac{\Gamma\left(\lambda + \frac{1}{2}\right)}{\sqrt{\pi}\,\Gamma(\lambda + 1)}, \quad x = \frac{\sqrt{8(\lambda+1)\theta_0^2 - 1}}{4(\lambda+1)\theta_0}, \quad y = \frac{1}{4(\lambda+1)\theta_0}.$$

So, the corresponding differentiation formula is

$$(3.1.5) \quad f'(a) \cong D_n^h f(a) = \frac{2}{\pi h} \operatorname{Re}\left(\frac{\sigma}{\zeta} \left(f\Big(a + \frac{h}{2}\,\zeta\Big) - f\Big(a - \frac{h}{2}\,\zeta\Big) \right) \right),$$

with the dominant error term $\dfrac{h^4}{7680(\lambda+1)^2} f^{(5)}(a)$. Here $\zeta = \zeta_1$ and $\sigma = \sigma_1$.

In error analysis of this formula with respect to λ, we have to note that $|\zeta| = 1/\sqrt{2(\lambda+1)}$, so that the distance between the nodes in (3.1.5) depends on λ, i.e. $|h\zeta| = h/\sqrt{2(\lambda+1)}$. So, for comparing the formulas of the form (3.1.5) with respect to λ, we must take $h/\sqrt{2(\lambda+1)} = \overline{h} = \text{const}$. Then, we see that the dominant error term becomes $\dfrac{\overline{h}^4}{1920} f^{(5)}(a)$, i.e. it does not depend on λ. Of course, the total error $R(f)$ depends of λ, but that influence is negligible, especially for $\overline{h}$ sufficiently small.

Asymptotically, for λ sufficiently large, we can prove that

$$\zeta \to \xi\sqrt{\lambda} \qquad \text{and} \qquad \frac{\sigma}{\zeta} \to \frac{A\pi\sqrt{\lambda}}{2},$$

where

$$\xi = \frac{\sqrt{8-\pi} + i\sqrt{\pi}}{4} \qquad \text{and} \qquad A = \frac{6-\pi}{\sqrt{8-\pi}} - \frac{i(\pi-2)}{\sqrt{\pi}}.$$

Then, we get the following differentiation formula

$$f'(a) \cong \frac{1}{h} \operatorname{Re}\left\{ A\left(f\Big(a + \frac{h}{2}\xi\Big) - f\Big(a - \frac{h}{2}\xi\Big)\right)\right\}. \tag{3.1.6}$$

Example 3.1.1. $f(z) = e^z/(\sin^3 z + \cos^3 z)$, $a = 0$, $n = 2$.

Using $\overline{h} = h|\zeta| = 2^{-k}$, $k = 0(1)5$, and $\lambda = 0$, $1/2$, 1 and 50, we obtain the approximations for $f'(0) = 1$, with errors given in Table 3.1.1. In the last column of this table we give the corresponding errors of the asymptotic formula (3.1.6). The above comments are evident from Table 3.1.1.

Table 3.1.1: Absolute errors in differentiation formula

k	$\overline{h}$	$\lambda = 0$	$\lambda = 1/2$	$\lambda = 1$	$\lambda = 50$	$\lambda \to \infty$
0	1	1.58(−1)	1.34(−1)	1.23(−1)	9.58(−2)	4.48(−2)
1	0.5	6.36(−3)	6.11(−3)	5.98(−3)	5.60(−3)	5.59(−3)
2	0.25	3.49(−4)	3.46(−4)	3.44(−4)	3.38(−4)	3.38(−4)
3	0.125	2.11(−5)	2.10(−5)	2.10(−5)	2.09(−5)	2.09(−5)
4	0.0625	1.31(−6)	1.31(−6)	1.31(−6)	1.30(−6)	1.30(−6)
5	0.03125	8.15(−8)	8.15(−8)	8.15(−8)	8.15(−8)	8.15(−8)

Similarly as in Ref. [22], some improvements for real-valued functions could be done. Also, the corresponding formulas for higher derivatives may be considered.

3.2 Cauchy Principal Values Integral

In this section we consider the Cauchy principal value integral

$$I_\lambda(\xi; f) = \fint_{-1}^{1} \frac{w(t)f(t)}{t-\xi}\, dt\,, \tag{3.2.1}$$

where $-1 < \xi < 1$ and $w(t) = (1-t^2)^{\lambda-1/2},\ \lambda > -1/2$. There are many ways of evaluating a singular integral of the type of (3.2.1) by numerical methods (see, for example, Refs. [5], [16], [17], [18], [23], [25], [26], [33]).

Here, we will show an application of our formula (2.1.1) to evaluation of the integral (3.2.1). Firstly, using the following linear fractional transformation $t = (x+\xi)/(x\xi+1)$, we obtain

$$I_\lambda(\xi; f) = w(\xi) \fint_{-1}^{1} w(x)\frac{g(\xi,x)}{x}\, dx\,,$$

where

$$g(\xi,x) = \frac{f\left(\dfrac{x+\xi}{x\xi+1}\right)}{(x\xi+1)^{2\lambda}}\,.$$

Let $D_+ = \{z \in \mathbb{C} : |z| < 1,\ \mathrm{Im}\, z > 0\}$. We assume that f is a regular analytic function on the closed upper unit half disc $\overline{D}_+$. Also, let $C_\varepsilon,\ 0 < \varepsilon < 1$, be the contour formed by ∂D_+, with small circular parts of radius ε and centers at ± 1 and origin spared out. Then, by Cauchy's theorem

$$0 = \int_{C_\varepsilon} \Psi(z)\, dz = \int\limits_{\gamma_{1,0}\cup\gamma_{\varepsilon,-1}\cup\gamma_{\varepsilon,+1}} \Psi(z)\, dz + \int\limits_{\gamma_{\varepsilon,0}} \Psi(z)\, dz + \int\limits_{[-1+\varepsilon,-\varepsilon]\cup[\varepsilon,1-\varepsilon]} \Psi(z)\, dz,$$

where $\gamma_{r,c}$ is a circular part of C_ε with radius r and center at C, and $\Psi(z) = w(z)g(\zeta,z)/z$.

Since $\lim\limits_{\varepsilon\to 0} \int_{\gamma_{\varepsilon,\pm1}} \Psi(z)\, dz = 0$ and

$$\lim_{\varepsilon\to 0} \int_{\gamma_{\varepsilon,0}} \Psi(z)\, dz = -i\pi \operatorname*{Res}_{z=0} \left\{ w(z)\frac{g(\zeta,z)}{z} \right\} = -i\pi g(\zeta,0) = -i\pi f(\zeta)\,,$$

letting $\varepsilon \to 0$, we obtain

$$\fint_{-1}^{1} \Psi(x)\, dx = i\pi f(\zeta) - \int_\Gamma \Psi(z)\, dz\,,$$

where $\Gamma = \left\{ z \in \mathbb{C} : z = e^{i\theta},\ 0 \le \theta \le \pi \right\}$.

If $f(z)$ is real for real z, we have

$$\fint_{-1}^{1} \Psi(x)\,dx = \operatorname{Im} \int_0^{\pi} w\left(e^{i\theta}\right) g\left(\zeta, e^{i\theta}\right)\, d\theta\,.$$

Applying (2.1.1) to the integral on the right yields

$$\fint_{-1}^{1} \Psi(x)\,dx = \operatorname{Im}\left\{\sum_{\nu=1}^{n} \sigma_\nu g(\zeta,\zeta_\nu) + R_n(g)\right\}\,.$$

So, we obtain

$$I_\lambda(\xi;f) \cong Q_{n,\lambda}(\xi;f) = w(\xi) \operatorname{Im} \sum_{\nu=1}^{n} \sigma_\nu g(\xi,\zeta_\nu)\,. \tag{3.2.2}$$

If f is meromorphic with poles $p_\nu,\ \nu = 1,\ldots,m$, in D_+, then we can derive the following formula

$$I_\lambda(\xi;f) \cong w(\xi) \operatorname{Im}\left\{\sum_{\nu=1}^{n} \sigma_\nu g(\xi,\zeta_\nu) - 2\pi \sum_{\nu=1}^{m} \operatorname*{Res}_{z=p_\nu} \Psi(z)\right\}\,. \tag{3.2.3}$$

Table 3.2.1: Absolute errors for $\lambda = 0$

n	$a=5$			$a=0.1$		
	$\xi=0.25$	$\xi=0.90$	$\xi=0.99$	$\xi=0.25$	$\xi=0.90$	$\xi=0.99$
2	3.77(−5)	7.42(−4)	2.76(−3)	4.15(0)	5.50(0)	1.35(0)
3	1.07(−6)	1.22(−3)	1.62(−3)	1.29(1)	1.39(1)	2.38(0)
4	4.06(−8)	8.51(−4)	6.82(−4)	3.35(1)	1.55(2)	3.62(0)
5	1.58(−10)	4.65(−4)	3.12(−5)	1.80(1)	1.40(1)	5.25(0)
6	9.95(−11)	2.26(−4)	5.23(−4)	4.35(0)	8.87(0)	7.58(0)
7	3.04(−13)	1.03(−4)	8.21(−4)	1.12(1)	8.65(0)	1.21(1)
8	1.56(−14)	4.47(−5)	9.67(−4)	4.47(1)	1.14(1)	1.76(1)

EXAMPLE 3.2.1. $f(t) = 1/(t^2 + a^2)$; $a = 5,\ 0.1$; $\xi = 0.25,\ 0.90,\ 0.99$.
The exact value of $I_0(\xi;f)$ is $-\dfrac{\pi\xi}{a} \cdot \dfrac{1}{\sqrt{1 + a^2(a^2+\xi^2)}}$.

Using the formulas (3.2.2) and (3.2.3), for $a = 5$ and $a = 0.1$, respectively, we obtain the numerical results, which errors (in Chebyshev case $\lambda = 0$) are presented in Table 3.2.1. The formula (3.2.3) is not stable. In this case we can get somewhat more accurate results by "subtracting out" the singularity from $I_\lambda(\xi;f)$.

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