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Polynomials Orthogonal on the Semicircle*

WALTER GAUTSCHI AND GRADIMIR V. MILOVANOVIĆ

Department of Computer Sciences, Purdue University, West Lafayette, Indiana 47907, U.S.A. and Faculty of Electronic Engineering, Department of Mathematics, University of Niš, 18000 Niš, Yugoslavia

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Complex polynomials $\{\pi_k\}$, $\pi_k(z)=z^k+\cdots$, orthogonal with respect to the complex-valued inner product $(f,g)=\int_0^\pi f(e^{i\theta})g(e^{i\theta})d\theta$ are studied. By direct calculation of moment determinants it is shown that these polynomials exist uniquely. The three-term recurrence relation satisfied by these polynomials is obtained explicitly as well as their relationship with Legendre polynomials. It is shown that the zeros of π_n are all simple and are located in the interior of the upper unit half disc, distributed symmetrically with respect to the imaginary axis. They can be (and have been) computed as eigenvalues of a real nonsymmetric tridiagonal matrix. A linear second-order differential equation is obtained for $\pi_n(z)$ which has regular singular points at $z=1, -1, \infty$ (like Legendre's equation) and an additional regular singular point on the negative imaginary axis. Applications are discussed involving Gauss–Christoffel quadrature over the semicircle, numerical differentiation, and the computation of Cauchy principal value integrals.

1. INTRODUCTION

We study orthogonal polynomials relative to the inner product

$$(f,g)=\int_\Gamma (iz)^{-1}f(z)g(z)\,dz, \tag{1.1}$$

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

$$(f,g)=\int_0^\pi f(e^{i\theta})g(e^{i\theta})d\theta. \tag{1.1'}$$

Note that the second factor g is not conjugated, so that the inner product is not Hermitian. Nevertheless, the orthogonal polynomials can be viewed

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as being orthogonal with respect to the (complex-valued) moment functional

$$\mathscr{L}z^k = \mu_k, \qquad \mu_k = \int_0^\pi e^{ik\theta} d\theta = \pi, \qquad k=0,$$
$$= 2i/k, \qquad k \text{ odd}, \tag{1.2}$$
$$= 0, \qquad k \text{ even}, k \neq 0.$$

This moment functional is shown to be quasi-definite; it therefore generates a unique system of (monic, complex) polynomials $\{\pi_k\}$ satisfying

$$\begin{aligned} \deg \pi_k &= k, & k&=0, 1, 2,..., \\ (\pi_k, \pi_l) &= 0 & &\text{if } k \neq l, \\ &\neq 0 & &\text{if } k = l. \end{aligned} \tag{1.3}$$

It turns out, moreover, that $(\pi_k, \pi_k) > 0$ for $k = 0, 1, 2, \ldots$. Orthogonality could not be achieved if Γ were the complete circle, since in that case $(f, g) = 2\pi f(0)g(0)$. One could consider, however, arbitrary circular arcs. Also, weight functions other than the constant weight function in (1.1′) can be studied. Some results in this direction, involving Gegenbauer type weight functions, indeed have already been obtained, but they are not yet sufficiently complete for presentation at this time.

The paper is organized as follows. In Section 2 we develop preliminary material on moment determinants which is used to establish quasi-definiteness of the moment functional (1.2). Section 3 develops the three-term recurrence relation for the orthogonal polynomials and Section 4 their connection with Legendre polynomials. In Section 5 we discuss the zeros of the orthogonal polynomial π_n and show, in particular, that all are contained in the open half disc $D_+ = \{z \in \mathbb{C}: |z| < 1, \operatorname{Im} z > 0\}$. A second-order linear differential equation for π_n is obtained in Section 6. Section 7 deals with Gauss–Christoffel quadrature formulae for integration over the semicircle, which are applied to numerical differentiation and, in Section 8, to compute Cauchy principal value integrals.

2. Preliminaries on Moment Determinants

The purpose of this section is to evaluate the determinants

$$\Delta_n = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \vdots & \vdots & & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-2} \end{vmatrix}, \qquad \Delta_n' = \begin{vmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-2} & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n-1} & \mu_{n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_{n-1} & \mu_n & \cdots & \mu_{2n-3} & \mu_{2n-1} \end{vmatrix}, \tag{2.1}$$

where μ_k are the moments defined in (1.2). We first express these determinants in terms of the Hilbert-type determinants

$$\begin{aligned} &H_0=1, \qquad H_m=\det\left[\frac{1}{2i+2j-3}\right]_{i,j=1}^{m}, \\ &H'_0=1, \qquad H'_m=\det\left[\frac{1}{2i+2j-1}\right]_{i,j=1}^{m}, \end{aligned} \tag{2.2}$$

$m=1,2,3,\ldots.$

LEMMA 2.1. *We have*

$$\Delta_n=2^n H_{n/2}^2,\ n\ (\text{even})\geqslant 2; \qquad \Delta_n=2^{n-1}\pi H'^2_{(n-1)/2},\ n\ (\text{odd})\geqslant 1. \tag{2.3}$$

Proof. Let first n be even. By (1.2) and (2.1), after removing a factor $2i$ from each even-numbered row and column, we have

$$\Delta_n=(-1)^{n/2}\,2^n \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & 0 & \frac{1}{n-1} \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & \frac{1}{n-1} & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & 0 & \frac{1}{n+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \cdots & 0 & \frac{1}{2n-3} \\ \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \frac{1}{n+3} & \cdots & \frac{1}{2n-3} & 0 \end{vmatrix}, \qquad n \text{ even.} \tag{2.4}$$

Using Laplace expansion by columns numbered $1,3,\ldots,n-1$, one finds that only one non-zero contribution results, namely from the minor and cominor pair

$$\begin{pmatrix} 2 & 4 & 6 & \cdots & n \\ 1 & 3 & 5 & \cdots & n-1 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 3 & 5 & \cdots & n-1 \\ 2 & 4 & 6 & \cdots & n \end{pmatrix}. \tag{2.5}$$

Since the moment matrix is symmetric, and the sign associated with the pair (2.5) is $(-1)^{n^2/4}$, one immediately obtains the first relation in (2.3).

To prove the second relation, for n odd, we use Laplace expansion by columns 1, 3,..., n in

$$\Delta_n = (-1)^{(n-1)/2}\, 2^{n-1} \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & \frac{1}{n-2} & 0 \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & 0 & \frac{1}{n} \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & \frac{1}{n} & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ \frac{1}{n-2} & 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & \cdots & 0 & \frac{1}{2n-3} \\ 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & 0 & \cdots & \frac{1}{2n-3} & 0 \end{vmatrix}, \quad n \text{ odd.} \quad \blacksquare \tag{2.6}$$

LEMMA 2.2. *We have*

$$\begin{aligned} \Delta'_n &= 2^{n-1} i\pi H'_{n/2} H'_{(n-2)/2}, && n\,(\text{even}) \geqslant 2, \\ &= 2^n i H_{(n+1)/2} H_{(n-1)/2}, && n\,(\text{odd}) \geqslant 1. \end{aligned} \tag{2.7}$$

Proof. If n is even, then

$$\Delta'_n = (-1)^{(n-2)/2}\, 2^{n-1} i \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & \frac{1}{n-3} & 0 & 0 \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & 0 & \frac{1}{n-1} & \frac{1}{n+1} \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & \frac{1}{n-1} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \cdots & \frac{1}{2n-5} & 0 & 0 \\ \frac{1}{n-1} & 0 & \frac{1}{n+1} & 0 & \frac{1}{n+3} & \cdots & 0 & \frac{1}{2n-3} & \frac{1}{2n-1} \end{vmatrix}, \quad n \text{ even.} \tag{2.8}$$

Laplace expansion by columns 1, 3, 5,..., $n-1$, n results in a single non-vanishing term, namely

$$\begin{pmatrix} 1 & 2 & 4 & \cdots & n-2 & n \\ 1 & 3 & 5 & \cdots & n-1 & n \end{pmatrix} \times \begin{pmatrix} 3 & 5 & 7 & \cdots & n-1 \\ 2 & 4 & 6 & \cdots & n-2 \end{pmatrix},$$

with sign $1+1+3+5+\cdots+(n-1)=(n^2+4)/4$, from which the first relation in (2.7) follows readily. The second relation follows similarly, using Laplace expansion by columns 2, 4,..., $n-1$, n in

$$\Delta'_n = (-1)^{(n-1)/2}\, 2^n i \cdot \begin{vmatrix} \pi & 1 & 0 & \frac{1}{3} & 0 & \cdots & 0 & \frac{1}{n-2} & \frac{1}{n} \\ 1 & 0 & \frac{1}{3} & 0 & \frac{1}{5} & \cdots & \frac{1}{n-2} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{5} & 0 & \cdots & 0 & \frac{1}{n} & \frac{1}{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ \frac{1}{n-2} & 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & \cdots & \frac{1}{2n-5} & 0 & 0 \\ 0 & \frac{1}{n} & 0 & \frac{1}{n+2} & 0 & \cdots & 0 & \frac{1}{2n-3} & \frac{1}{2n-1} \end{vmatrix}, \quad n \text{ odd.} \quad \blacksquare \tag{2.9}$$

In order to evaluate the determinants in (2.2), we use Cauchy's formula (Muir [11, p. 345])

$$\det\left[\frac{1}{a_i+b_j}\right]_{i,j=1}^{m} = \frac{\prod_{i>j=1}^{m} (a_i-a_j)(b_i-b_j)}{\prod_{i,j=1}^{m} (a_i+b_j)}. \tag{2.10}$$

LEMMA 2.3. *We have*

$$H_m = \frac{2^{2m^2-m} \prod_{k=1}^{2m-1} k! \prod_{k=1}^{m-1} (2k)!}{\prod_{k=1}^{m} (2m+2k-2)!}, \qquad m=1,2,3,..., \tag{2.11}$$

$$H'_m = \frac{2^{2m^2-m} \prod_{k=1}^{2m} k! \prod_{k=1}^{m} (2k)!}{m!^2 \prod_{k=1}^{m} (2m+2k)!}, \qquad m=1,2,3,.... \tag{2.12}$$

Proof. Use (2.10) with $a_i=2i$, $b_j=2j-3$, and simplify, to get (2.11). Similarly, (2.12) follows from (2.10) with $a_i=2i$, $b_j=2j-1$. $\blacksquare$

Combining Lemmas 2.1 and 2.3 yields

LEMMA 2.4. *We have*

$$\Delta_n = 2^{(n-1)^2}\pi \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n-1)/2} (2k)!^2}{((n-1)/2)!^4 \prod_{k=1}^{(n-1)/2} (n+2k-1)!^2}, \qquad n \text{ (odd)} \geqslant 1, \tag{2.13}$$

$$\Delta_n = 2^{n^2} \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n/2)-1} (2k)!^2}{\prod_{k=1}^{n/2} (n+2k-2)!^2}, \qquad n \text{ (even)} \geqslant 2. \tag{2.14}$$

Combining Lemmas 2.2 and 2.3 yields

LEMMA 2.5. *We have*

$$\Delta_n' = 2^{n^2} i \frac{\prod_{k=1}^{n-2} k!^2 \prod_{k=1}^{(n-1)/2} (2k)!^2}{(2n-1) \prod_{k=1}^{(n-1)/2} (n+2k-1)!^2}, \qquad n \text{ (odd)} \geqslant 1, \tag{2.15}$$

$$\Delta_n' = 2^{n^2-2n-1} i\pi \frac{n^2}{2n-1} \frac{\prod_{k=1}^{n-1} k!^2 \prod_{k=1}^{(n/2)-1} (2k)!^2}{(n/2)!^4 \prod_{k=1}^{(n/2)-1} (n+2k)!^2}, \qquad n \text{ (even)} \geqslant 2. \tag{2.16}$$

3. RECURRENCE RELATION

We note, first of all, from Lemma 2.4, that $\Delta_n > 0$, all $n \geqslant 1$, and therefore, in particular, that the moment sequence (1.2) is quasi-definite (cf., e.g., Chihara [2, Chap. 1, Definition 3.2]). The orthogonal polynomials (1.3) therefore exist uniquely, and $(\pi_k, \pi_k) = \Delta_{k+1}/\Delta_k > 0$ (Chihara [2, Chap. 1, Theorems 3.1 and 3.2]). Moreover, the following theorem holds.

THEOREM 3.1. *The (monic, complex) polynomials $\{\pi_k\}$ orthogonal with respect to the inner product* (1.1) *satisfy the recurrence relation*

$$\begin{gathered} \pi_{k+1}(z) = (z - i\alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z), \qquad k = 0, 1, 2, \ldots, \\ \pi_{-1}(z) = 0, \qquad \pi_0(z) = 1, \end{gathered} \tag{3.1}$$

where

$$\alpha_0 = \theta_0, \qquad \alpha_k = \theta_k - \theta_{k-1}, \qquad \beta_k = \theta_{k-1}^2, \qquad k \geqslant 1, \tag{3.2}$$

and θ_k is given by

$$\theta_k = \frac{2}{2k+1} \left[\frac{\Gamma((k+2)/2)}{\Gamma((k+1)/2)} \right]^2, \qquad k \geqslant 0. \tag{3.3}$$

Proof. The fact that the polynomials $\{\pi_k\}$ satisfy a three-term recurrence relation (3.1) follows from the property $(zf, g) = (f, zg)$ of the inner product (1.1) (cf. Gautschi [6, Theorem 2]). It is well-known that

$$\beta_k = \frac{\Delta_{k-1}\Delta_{k+1}}{\Delta_k^2}, \qquad k \geqslant 1, \tag{3.4}$$

from which the last relation in (3.2) follows via Lemma 2.4 by an elementary (but lengthy) computation. Likewise,

$$i\alpha_k = \frac{\Delta'_{k+1}}{\Delta_{k+1}} - \frac{\Delta'_k}{\Delta_k}, \qquad k \geqslant 0$$

(where $\Delta'_0 = 0$), from which the first two relations in (3.2) follow via Lemmas 2.4 and 2.5. ∎

Using Stirling's formula in (3.3), one finds from (3.2)

$$\alpha_k \to 0, \qquad \beta_k \to \tfrac{1}{4} \qquad \text{as } k \to \infty,$$

just like in Szegö's theory for orthogonal polynomials on the interval $[-1, 1]$ (Szegö [14, Eqs. (12.7.4) and (12.7.6)]).

From (3.1) and (3.2) it follows easily that $-i\theta_{k-1}$ is the coefficient of z^{k-1} in π_k,

$$\pi_k(z) = z^k - i\theta_{k-1} z^{k-1} + \cdots, \qquad k \geqslant 1. \tag{3.5}$$

Furthermore, $\|\pi_k\|^2 = \pi\beta_1\beta_2 \cdots \beta_k = \pi(\theta_0\theta_1 \cdots \theta_{k-1})^2$, by (3.2), and hence, by (3.3),

$$\|\pi_k\| = \frac{1}{\sqrt{\pi}} 2^{2k} \frac{k![\Gamma((k+1)/2)]^2}{(2k)!}, \qquad k \geqslant 0. \tag{3.6}$$

4. Connection with Legendre Polynomials

The polynomial π_n in (1.3) is simply related to the (monic) Legendre polynomials. We have, in fact,

THEOREM 4.1. *Let $\{\hat{P}_k\}$ denote the sequence of monic Legendre polynomials. Then the representation*

$$\pi_n(z) = \hat{P}_n(z) - i\theta_{n-1}\hat{P}_{n-1}(z), \qquad n \geqslant 1, \tag{4.1}$$

holds, where θ_k is given by (3.3).

Proof. Let $\hat{h}_k = \int_{-1}^{1} [\hat{P}_k(z)]^2 dz$. Then

$$\pi_n(z) = \gamma_0 \hat{P}_0(z) + \gamma_1 \hat{P}_1(z) + \cdots + \gamma_n \hat{P}_n(z),$$

where

$$\hat{h}_k \gamma_k = \int_{-1}^{1} \pi_n(z) \hat{P}_k(z)\, dz = -\int_0^{\pi} \pi_n(e^{i\theta}) \hat{P}_k(e^{i\theta}) ie^{i\theta} d\theta,$$

the second equality following from Cauchy's theorem. Since $z\hat{P}_k(z)$ is a linear combination of $\pi_0(z), \pi_1(z), \ldots, \pi_{k+1}(z)$, the orthogonality relations (1.3) yield $\gamma_0 = \gamma_1 = \cdots = \gamma_{n-2} = 0$. Clearly, $\gamma_n = 1$, while, in view of (3.5),

$$\begin{aligned}\hat{h}_{n-1}\gamma_{n-1} &= \int_{-1}^{1} (z^n - i\theta_{n-1} z^{n-1} + \cdots) \hat{P}_{n-1}(z) dz \\ &= \int_{-1}^{1} z^n \hat{P}_{n-1}(z) dz - i\theta_{n-1} \hat{h}_{n-1}.\end{aligned}$$

Here the second integral vanishes, the integrand being an odd function, and so $\gamma_{n-1} = -i\theta_{n-1}$. ∎

5. The Zeros of $\pi_n(z)$

We begin with a simple symmetry property.

THEOREM 5.1. *If $\zeta \in \mathbb{C}$ is a zero of the polynomial π_n, then so is $-\bar{\zeta}$. The zeros of π_n are thus located symmetrically with respect to the imaginary axis.*

Proof. Denote by $\bar{\pi}_n$ the polynomial obtained from π_n by conjugating all coefficients,

$$\bar{\pi}_n(z) = \overline{\pi_n(\bar{z})}.$$

Equation (4.1) then shows that

$$\pi_n(-z) = (-1)^n \bar{\pi}_n(z). \tag{5.1}$$

Therefore, if ζ is a zero of π_n, there follows

$$0 = \pi_n(\zeta) = (-1)^n \bar{\pi}_n(-\zeta) = (-1)^n \overline{\pi_n(-\bar{\zeta})},$$

hence $\pi_n(-\bar{\zeta}) = 0$. ∎

We show next that all zeros of π_n lie in the upper unit half disc.

THEOREM 5.2. *All zeros of the polynomial* π_n *are contained in* $D_+ = \{z \in \mathbb{C}: |z| < 1 \text{ and} \operatorname{Im} z > 0\}$.

Proof. We first apply Rouché's theorem to show that all zeros of π_n lie in the open unit disc $D = \{z \in \mathbb{C}: |z| < 1\}$. Consider

$$Q_n(z) = \frac{\hat{P}_n(z)}{\hat{P}_{n-1}(z)}, \qquad z \in \partial D.$$

We are seeking lower bounds q_n (not depending on z) of $|Q_n(z)|$ for $z \in \partial D$,

$$|Q_n(z)| \geqslant q_n, \qquad z \in \partial D.$$

From the recurrence relation for the (monic) Legendre polynomials

$$\hat{P}_n(z) = z\hat{P}_{n-1}(z) - \frac{1}{4-(n-1)^{-2}} \hat{P}_{n-2}(z),$$

we find

$$Q_n(z) = z - \frac{1}{4-(n-1)^{-2}} \frac{1}{Q_{n-1}(z)}. \tag{5.2}$$

Since $Q_1(z) = z$, we clearly have $q_1 = 1$. Furthermore, (5.2) shows that we can take

$$q_1 = 1, \qquad q_n = 1 - \frac{1}{4-(n-1)^{-2}} \frac{1}{q_{n-1}}, \qquad n \geqslant 2.$$

It is readily seen by induction that

$$q_n = \frac{n}{2n-1}, \qquad n \geqslant 1.$$

Therefore, $|\hat{P}_n(z)| \geqslant (n/(2n-1))|\hat{P}_{n-1}(z)|$ on ∂D, and thus

$$|\hat{P}_n(z)| \geqslant \frac{n}{2n-1} \frac{1}{\theta_{n-1}} |\theta_{n-1} \hat{P}_{n-1}(z)|, \qquad z \in \partial D,$$

where θ_k is given in (3.3). Now,

$$\frac{n}{2n-1} \frac{1}{\theta_{n-1}} = \frac{2}{n} \left[\Gamma\left(\frac{n}{2}+1\right) \Big/ \Gamma\left(\frac{n+1}{2}\right) \right]^2,$$

and using a refinement of Gautschi's inequality for the gamma function,

$$\frac{\Gamma(x+1)}{\Gamma(x+s)} > (x + \tfrac{1}{2}s)^{1-s}, \qquad x > 0, 0 < s < 1,$$

due to Kershaw [10], with $x=n/2$, $s=\frac{1}{2}$, one finds

$$\frac{n}{2n-1}\frac{1}{\theta_{n-1}}>\frac{2n+1}{2n}>1. \tag{5.3}$$

Consequently, $|\hat{P}_n(z)|>|\theta_{n-1}\hat{P}_{n-1}(z)|$ on ∂D, and therefore by Rouché's theorem, applied to (4.1), all zeros of π_n lie in D.

To complete the proof of Theorem 5.2 we use in (4.1) a result of Giroux [8, Corollary 3], according to which all zeros of π_n either lie in the half strip $\operatorname{Im} z\geqslant 0$, $-\xi_n\leqslant \operatorname{Re} z\leqslant \xi_n$, or in the conjugate half strip, where ξ_n is the largest zero of the Legendre polynomial P_n. Since by (3.5) the sum of the zeros has positive imaginary part, it is the upper half strip that applies. It remains to show that all zeros of π_n are nonreal. If there were a zero $\zeta=x\in\mathbb{R}$, then indeed $\hat{P}_{n-1}(x)\neq 0$, since otherwise, by (4.1), we would have the contradiction $\hat{P}_n(x)=\hat{P}_{n-1}(x)=0$. The same equation (4.1) then implies $i\theta_{n-1}=\hat{P}_n(x)/\hat{P}_{n-1}(x)$, which is plainly impossible. ∎

Remarks. (1) We have proved, more precisely, that all zeros of π_n are contained in the region $\{z\in\mathbb{C}\colon |z|<1\}\cap\{z\in\mathbb{C}\colon \operatorname{Im} z>0,\ -\xi_n\leqslant \operatorname{Re} z\leqslant\xi_n\}$, where ξ_n is the largest zero of the Legendre polynomial P_n.

(2) The fact that all zeros of π_n lie in the closure of D follows also from a result of Specht [13, Satz 7*], applied to (4.1), and Kershaw's inequality used above. We feel, however, that our proof has independent interest.

THEOREM 5.3. *All zeros of π_n are simple.*

Proof. Let ζ be a zero of π_n, hence, by (4.1),

$$\hat{P}_n(\zeta)=i\theta_{n-1}\hat{P}_{n-1}(\zeta).$$

We prove that $\pi_n'(\zeta)\neq 0$.

Using the recurrence relations

$$\hat{P}_{k+1}(z)=z\hat{P}_k(z)-\frac{k^2}{4k^2-1}\hat{P}_{k-1}(z) \tag{5.4}$$

and

$$(1-z^2)\,\hat{P}_k'(z)=(k+1)\,z\hat{P}_k(z)-(2k+1)\,\hat{P}_{k+1}(z) \tag{5.5}$$

in

$$\pi_n'(\zeta)=\hat{P}_n'(\zeta)-i\theta_{n-1}\hat{P}_{n-1}'(\zeta)=\frac{1}{\hat{P}_{n-1}(\zeta)}\,[\hat{P}_n'(\zeta)\hat{P}_{n-1}(\zeta)-\hat{P}_n(\zeta)\hat{P}_{n-1}'(\zeta)]$$

yields, after a little computation,

$$\pi_n'(\zeta)=\frac{1}{(1-\zeta^2)\hat{P}_{n-1}(\zeta)}\left[\frac{n^2}{2n-1}\hat{P}_{n-1}^2(\zeta)+(2n-1)\hat{P}_n^2(\zeta)-2n\zeta\hat{P}_n(\zeta)\hat{P}_{n-1}(\zeta)\right]$$
$$=\frac{\hat{P}_{n-1}(\zeta)}{(1-\zeta^2)(2n-1)}\left[n^2-(2n-1)^2\theta_{n-1}^2-2n(2n-1)\zeta\theta_{n-1}i\right].$$

Letting $\zeta=\alpha+i\beta$, the expression in brackets becomes

$$n^2-(2n-1)^2\theta_{n-1}^2+2n(2n-1)\beta\theta_{n-1}-2n(2n-1)\alpha\theta_{n-1}i,$$

which, by virtue of $\beta>0$ and (5.3), is clearly nonzero. ∎

The zeros ζ_ν of π_n may be computed as eigenvalues of the Jacobi matrix

$$J_n=\begin{bmatrix} i\alpha_0 & \theta_0 & & & 0 \\ \theta_0 & i\alpha_1 & \theta_1 & & \\ & \theta_1 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ 0 & & & \theta_{n-2} & i\alpha_{n-1} \end{bmatrix}. \tag{5.6}$$

By a similarity transformation with the diagonal matrix $D_n=\operatorname{diag}(1, i, i^2, i^3, 1, i, \ldots)\in\mathbb{R}^{n\times n}$ these can be seen to equal $\zeta_\nu=i\eta_\nu$, where η_ν are the eigenvalues of the real nonsymmetric tridiagonal matrix

$$-iD_n^{-1}J_nD_n=\begin{bmatrix} \alpha_0 & \theta_0 & & & 0 \\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ 0 & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix}. \tag{5.7}$$

Using the EISPACK routine HQR [12, p. 240], we computed all zeros of π_n for selected values of n up to $n=73$. Figure 1 shows those with non-negative real parts for $n=2(1)11$, as well as those with smallest, and next to smallest, positive real parts for $n=12, 16, 24, 40, 72$ and those with smallest positive real parts for $n=13, 17, 25, 41, 73$.

Figure 1, together with the facts that $\pi_1(z)=z-(2i/\pi)$ and $\pi_3(z)=z^3-(8i/5\pi)z^2-(3/5)z+(8i/15\pi)$, suggests that the imaginary part of every zero of π_n is $\leqslant 2/\pi$, if $n\geqslant 1$, and $\leqslant .315076\ldots$, the unique positive root of $t^3-(8/5\pi)t^2+(3/5)t-(8/15\pi)=0$, if $n\geqslant 2$.

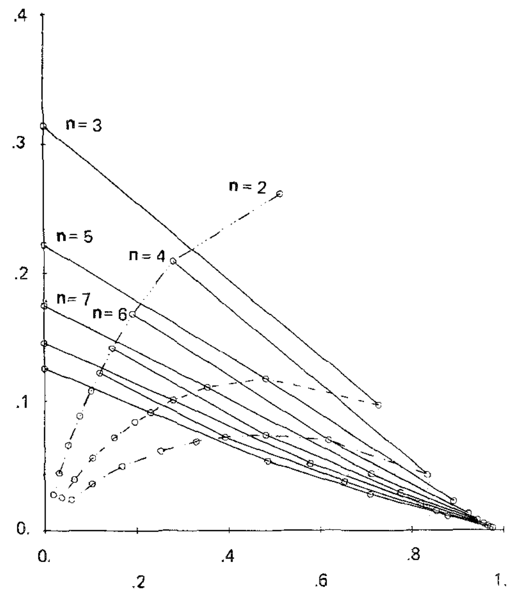

FIGURE 1

6. Differential Equation

Like the Legendre polynomial P_n, the polynomial π_n satisfies a second-order linear differential equation with regular singular points at $1, -1, \infty$. There is, however, an additional regular singular point on the negative imaginary axis which moves as a function of n.

THEOREM 6.1. *The polynomial $\pi_n(z)$ satisfies the differential equation*

$$\begin{aligned}(1-z^2)\,[n^2-(2n-1)^2\theta_{n-1}^2-2n(2n-1)zi\theta_{n-1}]\pi_n''(z)\\ -2[(n^2-(2n-1)^2\theta_{n-1}^2)z-n(2n-1)(z^2+1)i\theta_{n-1}]\pi_n'(z) \qquad (6.1)\\ +n[(n+1)n^2-(n-1)(2n-1)^2\theta_{n-1}^2-2(2n-1)n^2zi\theta_{n-1}]\pi_n(z)=0,\end{aligned}$$

where θ_k is given by (3.3).

Proof[1]. Let $u=\hat{P}_{n-1}(z)$ and $v=(2n-1)\pi_n(z)$, and define

$$\omega(z)=(z-1)^{(n/2)-(n-1/2)i\theta_{n-1}}(z+1)^{(n/2)+(n-1/2)i\theta_{n-1}}, \qquad (6.2)$$

[1] The authors are indebted to Professor F. Calogero for the reference Ahmed and Bruschi [1], where similar proof techniques are employed.

where we assume, for the moment, that $z \in D_+ = \{z \in \mathbb{C}: |z| < 1$ and $\operatorname{Im} z > 0\}$ and where fractional and imaginary powers denote principal branches. An elementary calculation, using (5.5) and (4.1), will show that

$$(z^2-1)[\omega(z)u]' = \omega(z)v, \tag{6.3}$$

where the prime denotes differentiation with respect to z. There follows

$$u = \frac{1}{\omega}\int \frac{\omega}{z^2-1}\, v\,dz,$$

$$u' = \left(\frac{1}{\omega}\right)' \int \frac{\omega}{z^2-1}\, v\,dz + \frac{1}{z^2-1}\, v,$$

$$u'' = \left(\frac{1}{\omega}\right)'' \int \frac{\omega}{z^2-1}\, v\,dz + \left(\frac{1}{\omega}\right)' \frac{\omega}{z^2-1}\, v + \left(\frac{1}{z^2-1}\right)' v + \frac{1}{z^2-1}\, v'.$$

Inserting this into Legendre's differential equation

$$(z^2-1)u'' + 2zu' - n(n-1)u = 0,$$

and simplifying, yields

$$v' - \frac{\omega'}{\omega}\, v + \left[\left((z^2-1)\left(\frac{1}{\omega}\right)'\right)' - \frac{n(n-1)}{\omega}\right] \int \frac{\omega}{z^2-1}\, v\,dz = 0. \tag{6.4}$$

Noting by (6.2) that

$$-\frac{\omega'}{\omega} = \frac{-nz + (2n-1)i\theta_{n-1}}{z^2-1} =: a(z),$$

$$\left((z^2-1)\left(\frac{1}{\omega}\right)'\right)' - \frac{n(n-1)}{\omega} = \frac{1}{\omega}\,\frac{n^2-(2n-1)^2\theta_{n-1}^2 - 2n(2n-1)zi\theta_{n-1}}{z^2-1}$$

$$=: b(z), \tag{6.5}$$

one obtains from (6.4)

$$\frac{1}{b(z)}\, v' + \frac{a(z)}{b(z)}\, v + \int \frac{\omega}{z^2-1}\, v\,dz = 0.$$

Differentiating this with respect to z and multiplying the result by $-[n^2-(2n-1)^2\theta_{n-1}^2 - 2n(2n-1)zi\theta_{n-1}]^2/\omega(z)$ yields, after some lengthy, but elementary computation, the desired differential equation (6.1). By the permanence principle, the restriction imposed on z can now be lifted. ∎

We remark that the differential equation (6.1) has four regular singular points, one each at $1, -1$, and ∞, and an additional one at $z_0 = -[n^2 - (2n-1)^2\theta_{n-1}^2]i/[2n(2n-1)\theta_{n-1}]$. In view of (5.3), z_0 is located on the negative imaginary axis; it approaches the origin monotonically as n increases. Since by Theorem 5.2 the zeros of π_n are contained in D_+, and therefore are regular points of the differential equation (6.1), it follows again that they must all be simple.

7. Gauss–Christoffel Quadrature over the Semicircle

The orthogonal polynomials $\pi_n(z)$ can be used in the usual way (see, e.g., Gautschi [7, Section 1.3]) to construct a Gauss–Christoffel quadrature rule

$$\int_0^\pi g(e^{i\theta})d\theta = \sum_{\nu=1}^{n} \sigma_\nu g(\zeta_\nu) + R_n(g), \qquad R_n(\mathbf{P}_{2n-1}) = 0, \tag{7.1}$$

for integrals over the semicircle. Indeed, the nodes $\zeta_\nu = \zeta_\nu^{(n)}$ are precisely the zeros of $\pi_n(z)$, whereas the weights $\sigma_\nu = \sigma_\nu^{(n)}$ can be obtained by an adaptation of the procedure of Golub and Welsch [9]. Letting $\tilde{\pi}_k(z) = \pi_k(z)/\|\pi_k\|$ denote the normalized orthogonal polynomials and

$$\tilde{\pi}(z) = [\tilde{\pi}_0(z), \tilde{\pi}_1(z), ..., \tilde{\pi}_{n-1}(z)]^T$$

the vector of the first n of them, it is easily seen that

$$J_n \tilde{\pi}(\zeta_\nu) = \zeta_\nu \tilde{\pi}(\zeta_\nu),$$

where J_n is the Jacobi matrix in (5.6). The nodes ζ_ν are therefore the eigenvalues of J_n and $\tilde{\pi}(\zeta_\nu)$ the corresponding eigenvectors. Defining

$$p(z) = D_n^{-1} \tilde{\pi}(z), \tag{7.2}$$

where, as before, $D_n = \text{diag}\,(1, i, i^2, i^3, 1, i, ...)$, one finds

$$[-iD_n^{-1} J_n D_n] p(\zeta_\nu) = \eta_\nu p(\zeta_\nu), \tag{7.3}$$

i.e., $p(\zeta_\nu)$ is an eigenvector of the real matrix (5.7) corresponding to the eigenvalue $\eta_\nu = -i\zeta_\nu$. Denote by V_n the matrix of the eigenvectors of (5.7), each normalized so that the first component is equal to 1. Then

$$V_n = [v_1, v_2, ..., v_n], \qquad v_\nu = \sqrt{\pi}\, p(\zeta_\nu). \tag{7.4}$$

Now substituting in (7.1) for g in turn all components of the vector $p(z)$ in (7.2) yields

$$\sqrt{\pi} e_1 = \frac{1}{\sqrt{\pi}} V_n \sigma, \qquad \sigma = [\sigma_1, \sigma_2, ..., \sigma_n]^T,$$

where e_1 is the first coordinate vector. Therefore,

$$V_n \sigma = \pi e_1. \tag{7.5}$$

The weights σ_ν in (7.1) can thus be found by solving the linear system of equations (7.5). Using the EISPACK routine HQR2 [12, p. 248] to compute the matrix V_n, and the LINPACK routines CGECO and CGESL [4, Chap. 1] to solve the system (7.5), we observed estimates of the condition number (furnished by CGECO) which were only moderately large. For example, cond $V_n = 20.5, 73.3, 184.9$ for $n = 10, 20, 40$, respectively. It thus appears that the system (7.5) is reasonably well conditioned.

Since the matrix in (7.3) is real, the nonreal eigenvalues η_ν occur in conjugate complex pairs (see also Theorem 5.1). One has, moreover, the following theorem.

THEOREM 7.1. *If η_ν is real, so is σ_ν. If $\eta_{\nu+1} = \bar{\eta}_\nu$ is complex, then $\sigma_{\nu+1} = \bar{\sigma}_\nu$.*

Proof. Assume first that n is odd, and for simplicity, that there is one real eigenvalue η_1 and $n-1$ conjugate complex eigenvalues $\eta_{2\nu+1} = \bar{\eta}_{2\nu}$, $\nu = 1, 2, ..., [n/2]$. (Figure 1 suggests that this is indeed the case.) Then the first eigenvector v_1 in (7.4) is real and the others occur in conjugate complex pairs, $v_{2\nu+1} = \bar{v}_{2\nu}$, $\nu = 1, 2, ..., [n/2]$. By (7.5) therefore,

$$\sigma_1 v_1 + \sum_{\nu=1}^{[n/2]} (\sigma_{2\nu} v_{2\nu} + \sigma_{2\nu+1} \bar{v}_{2\nu}) = \pi e_1.$$

Conjugating this, gives

$$\sigma_1 v_1 + \sum_{\nu=1}^{[n/2]} (\bar{\sigma}_{2\nu+1} v_{2\nu} + \bar{\sigma}_{2\nu} \bar{v}_{2\nu}) = \pi e_1.$$

By the nonsingularity of V_n, hence the uniqueness of σ, there follows $\sigma_{2\nu+1} = \bar{\sigma}_{2\nu}$ for $\nu = 1, 2, ..., [n/2]$, proving the second part of the theorem. Since the sum above, as well as v_1, are real, it follows that also σ_1 is real, which proves the first part of the theorem. A similar argument applies when n is even. ∎

In Table I we display the Gauss–Christoffel formulae (to 8 decimals only, to save space) for $n = 5, 10, 20$. They were obtained (to higher precision) on the CDC 6500 computer, using the routines HQR2, CGECO and CGESL mentioned above.

EXAMPLE 7.1. $\int_0^\pi \exp(ce^{i\theta})d\theta = \pi + i[Ei(c) + E_1(c)]$, $c > 0$.

The exact answer in terms of the exponential integrals (cf. Gautschi and Cahill [5, Eqs. 5.1.1 and 5.1.2]) follows from (8.1) below (where $f(z) = \exp(cz)$) and (8.8) (where $x = 0$).

We apply the Gauss–Christoffel rule (7.1) with $g(z) = \exp(cz)$ for $n = 2, 5, 10, 20$ and $c = .2, .6, 1.0, 2.0, 6.0, 10.0$. The results are compared with the approximations furnished by the composite trapezoidal rule based on n equal subintervals of $[0, \pi]$ and by the n-point Gauss–Legendre formula on $[0, \pi]$. Since the real part of the integrand is an even function, the trapezoidal rule must produce for the real part half of the result it would obtain if it were applied over the whole interval of periodicity, $[-\pi, \pi]$, using $2n$ subintervals. In particular, the composite trapezoidal rule, like the Gauss–Christoffel rule (7.1), integrates the first $2n-1$ powers in the real part exactly. This will not be the case for the imaginary part, which is an odd function. Here the trapezoidal rule, unlike the Gauss rule, integrates

TABLE I

Gauss–Christoffel Formula for $n = 5, 10, 20$

n	ν	ζ_ν		σ_ν	
5	1,2	± 0.89052727	$+0.022495461i$	0.0072402551	$\pm 0.30663646i$
	3,4	± 0.48026508	$+0.11792794i$	0.50270345	$\pm 0.92618932i$
	5		$0.22216141i$	1.99138066	
10	1,2	± 0.97146604	$+0.0028731070i$	0.0078107581	$\pm 0.074979250i$
	3,4	± 0.85284258	$+0.015150376i$	0.023571055	$\pm 0.19000917i$
	5,6	± 0.65232339	$+0.037578303i$	0.063357456	$\pm 0.35652707i$
	7,8	± 0.39255204	$+0.072381390i$	0.23196483	$\pm 0.66539219i$
	9,10	± 0.11928205	$+0.12236097i$	1.24409223	$\pm 0.83467375i$
20	1,2	± 0.99279481	$+0.00036088122i$	0.00093961488	$\pm 0.018602063i$
	3,4	± 0.96223284	$+0.0019015682i$	0.0023283767	$\pm 0.044211071i$
	5,6	± 0.90804700	$+0.0046758976i$	0.0041099345	$\pm 0.072223615i$
	7,8	± 0.83157445	$+0.0086981042i$	0.0066940217	$\pm 0.10457986i$
	9,10	± 0.73472727	$+0.014013039i$	0.010908872	$\pm 0.14441960i$
	11,12	± 0.61995356	$+0.020739446i$	0.018712830	$\pm 0.19743837i$
	13,14	± 0.49022929	$+0.029167472i$	0.035680664	$\pm 0.27542598i$
	15,16	± 0.34918044	$+0.040007722i$	0.082367746	$\pm 0.40649151i$
	17,18	± 0.20200473	$+0.055045977i$	0.26876888	$\pm 0.65608704i$
	19,20	± 0.061601584	$+0.075471956i$	1.14028539	$\pm 0.69192546i$

exactly only linear terms, and the error in the imaginary part must be expected to exhibit the familiar $\mathcal{O}(h^2)$ behavior, where $h=\pi/n$. Table II shows the results (numbers in parentheses denote decimal exponents). The three pairs of entries for each c and n represent the relative errors in the real and imaginary part corresponding to the n-point Gauss–Christoffel rule (7.1), the n-point Gauss–Legendre rule on $[0, \pi]$, and the composite $(n+1)$-point trapezoidal rule, in that order. Note that the error of the Gauss–Christoffel rule, even for the real part, is usually several orders of magnitude smaller than the corresponding error of the trapezoidal rule, unless both are near the level of machine precision (3.553×10^{-15} on the CDC 6500 computer). The large errors of the trapezoidal rule in the imaginary parts, and their $\mathcal{O}(h^2)$ decay, are particularly conspicuous. Note also the relatively poor performance (compared to (7.1)) of the Gauss–Legendre rule.

The exponential integrals Ei and E_1 in Example 7.1 were computed by the FUNPACK functions *EI* and *EONE*, respectively (cf. Cody [3]).

EXAMPLE 7.2. $f'(a) = (1/\pi h) \int_0^\pi e^{-i\theta} [f(a+(h/2)e^{i\theta}) - f(a-(h/2)e^{i\theta})] d\theta.$

TABLE II

Relative Errors in Real and Imaginary Parts

c		$n=2$		$n=5$		$n=10$		$n=20$	
0.2	GC	7.4(−6)	2.4(−6)	9.0(−15)	7.1(−14)	1.4(−14)	1.2(−13)	2.7(−14)	2.1(−13)
	GL	4.8(−3)	2.5(−2)	4.7(−7)	1.2(−5)	4.5(−14)	3.0(−12)	4.6(−13)	2.4(−13)
	T	6.7(−5)	2.2(−1)	1.4(−14)	3.4(−2)	1.4(−14)	8.4(−3)	2.7(−14)	2.1(−3)
0.6	GC	6.0(−4)	1.9(−4)	3.1(−12)	5.1(−13)	1.8(−14)	1.2(−13)	2.7(−14)	2.0(−13)
	GL	3.8(−2)	3.3(−2)	6.5(−5)	2.1(−5)	7.4(−11)	6.2(−10)	4.0(−13)	2.4(−13)
	T	5.4(−3)	2.8(−1)	1.7(−9)	3.9(−2)	2.3(−14)	9.6(−3)	3.2(−14)	2.4(−3)
1.0	GC	4.7(−3)	1.5(−3)	5.2(−10)	7.1(−11)	2.3(−14)	1.3(−13)	1.4(−14)	2.2(−13)
	GL	8.3(−2)	1.4(−1)	2.8(−4)	6.4(−4)	6.8(−9)	6.0(−9)	3.7(−13)	2.2(−13)
	T	4.2(−2)	3.7(−1)	2.8(−7)	5.0(−2)	1.4(−14)	1.2(−2)	5.0(−14)	3.0(−3)
2.0	GC	7.8(−2)	2.1(−2)	5.6(−7)	6.4(−8)	2.3(−14)	1.6(−13)	4.5(−15)	2.8(−13)
	GL	1.6(−1)	4.9(−1)	1.1(−2)	5.2(−3)	2.3(−7)	1.1(−6)	4.0(−13)	1.4(−13)
	T	6.7(−1)	7.1(−1)	2.8(−4)	1.1(−1)	3.9(−13)	2.5(−2)	5.4(−14)	6.2(−3)
6.0	GC	9.0(0)	6.0(−1)	5.3(−2)	1.1(−3)	4.0(−9)	4.2(−11)	1.0(−12)	8.7(−13)
	GL	4.9(1)	2.1(0)	1.3(1)	3.2(−1)	9.3(−2)	1.2(−3)	3.4(−8)	2.5(−11)
	T	1.0(2)	1.0(0)	1.7(1)	1.4(0)	1.5(−3)	2.6(−1)	3.4(−13)	5.9(−2)
10.0	GC	1.1(2)	1.0(0)	2.2(1)	2.8(−2)	2.0(−4)	1.2(−7)	5.9(−11)	1.6(−12)
	GL	1.3(3)	1.2(0)	6.4(2)	2.1(0)	8.2(1)	1.2(−2)	1.1(−4)	1.4(−6)
	T	5.5(3)	1.0(0)	2.8(3)	1.3(0)	4.1(1)	1.0(0)	1.2(−8)	1.9(−1)

Note. Gauss–Christoffel (GC), Gauss–Legendre (GL), and trapezoidal (T) integration of $\int_0^\pi \exp(ce^{i\theta}) d\theta$.

TABLE III

Numerical differentiation by (7.7) with $n=2$, for $f(z)=\exp(z)$, $a=0$

h	$f'(0)\approx$
1.	0.99994199437142
0.5	0.99999638098906
0.25	0.99999977391086
0.125	0.99999998587099
0.0625	0.99999999911702
0.03125	0.99999999994522
0.015625	0.99999999999667

It is assumed here that f is analytic on some domain containing the point a and a circular neighborhood of a with radius $h/2$. The formula given for the derivative is then an easy consequence of Cauchy's theorem. Applying (7.1) to the integral on the right yields

$$f'(a)\approx\frac{1}{\pi h}\sum_{\nu=1}^{n}\frac{\sigma_\nu}{\zeta_\nu}\left[f\left(a+\frac{h}{2}\zeta_\nu\right)-f\left(a-\frac{h}{2}\zeta_\nu\right)\right]. \tag{7.6}$$

In the case where a is real, and $f(z)$ is real for real z, this can be simplified by using Theorems 5.1 and 7.1. For example, when n is even, and $\operatorname{Re}\zeta_\nu>0$ for $\nu=1, 2,..., n/2$, one finds

$$f'(a)\approx\frac{2}{\pi h}\sum_{\nu=1}^{n/2}\operatorname{Re}\left\{\frac{\sigma_\nu}{\zeta_\nu}\left[f\left(a+\frac{h}{2}\zeta_\nu\right)-f\left(a-\frac{h}{2}\zeta_\nu\right)\right]\right\}, \qquad n \text{ even.} \tag{7.7}$$

To give a numerical illustration, let $f(z)=e^z$, $a=0$ and $n=2$. Then

$$\zeta_1=\frac{1}{12}\left[\sqrt{48-\pi^2}+i\pi\right], \qquad \sigma_1=\frac{1}{2}\left[\pi+i\frac{24-\pi^2}{\sqrt{48-\pi^2}}\right],$$

$$\frac{\sigma_1}{\zeta_1}=\frac{1}{4}\left[\pi\frac{36-\pi^2}{\sqrt{48-\pi^2}}+i(12-\pi^2)\right],$$

and (7.7) for $h=2^{-k}$, $k=0(1)6$, produces the approximations in Table III.

8. An Application to Cauchy Principal Value Integrals

Let C_ε, $0<\varepsilon<1$, be the contour in the complex plane formed by the unit upper semicircle, the line segment from -1 to $-\varepsilon$, the upper semicircle of radius ε and center at the origin, and the line segment from ε to 1. For any function f analytic on the closed upper unit half disc we then have, by Cauchy's theorem, $\lim_{\varepsilon \downarrow 0} \int_{C_\varepsilon} f(z)\, dz/z = 0$, hence

$$\fint_{-1}^{1} \frac{f(t)}{t}\, dt = i\left\{\pi f(0) - \int_0^\pi f(e^{i\theta})\, d\theta\right\}, \tag{8.1}$$

where the integral on the left is a Cauchy principal value integral. In particular, if $f(z)$ is real for real z, as we shall henceforth assume, we have

$$\fint_{-1}^{1} \frac{f(t)}{t}\, dt = \operatorname{Im} \int_0^\pi f(e^{i\theta})\, d\theta. \tag{8.2}$$

If the singularity is not at the origin, but at some arbitrary point x on $(-1, 1)$, we map x to the origin by a linear fractional transformation and obtain

$$\fint_{-1}^{1} \frac{f(t)}{t-x}\, dt = \fint_{-1}^{1} \frac{g(x, t)}{t}\, dt = \operatorname{Im} \int_0^\pi g(x, e^{i\theta})\, d\theta, \tag{8.3}$$

where

$$g(x, z) = f\frac{z+x}{xz+1}\bigg/(xz+1). \tag{8.4}$$

Applying (7.1) to (8.3) yields

$$\fint_{-1}^{1} \frac{f(t)}{t-x}\, dt = \operatorname{Im}\left\{\sum_{\nu=1}^{n} \sigma_\nu g(x, \zeta_\nu) + R_n(g(x, \cdot))\right\}. \tag{8.5}$$

Note that $g(x, z)$ has a singularity at $z = -1/x$, which is farther away from the interval $[-1, 1]$ the smaller $|x|$. We expect therefore (8.5) to provide a good approximation (when R_n is neglected), unless $|x|$ is close to 1.

One might think of proceeding more directly by following the derivation at the beginning of this section, but with a contour C_ε that excludes the point x rather than 0. This would give

$$\fint_{-1}^{1} \frac{f(t)}{t-x}\, dt = i\left\{\pi f(x) - \int_0^\pi \frac{f(e^{i\theta})}{1 - xe^{-i\theta}}\, d\theta\right\}, \qquad -1 < x < 1. \tag{8.6}$$

Applying the quadrature rule (7.1) to the integral on the right of (8.6), however, would produce poor results, owing to the pole at $z = x$ of the integrand function $f(z)/(1 - xz^{-1})$.

A better alternative is to use Gauss–Legendre quadrature on (8.3) (cf., e.g., Gautschi [7, p. 106]),

$$\int_{-1}^{1} \frac{f(t)}{t-x}\, dt \approx \sum_{\nu=1}^{n} \frac{\lambda_\nu}{\tau_\nu} g(x, \tau_\nu), \qquad n \text{ even}, \tag{8.7}$$

where $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the Legendre polynomial P_n and $\lambda_\nu = \lambda_\nu^{(n)}$ the associated Christoffel numbers. This requires only real arithmetic, in contrast to (8.5), but may be less stable on account of the division by the two zeros τ_ν of opposite sign closest to the origin.

EXAMPLE 8.1. $I(x, c) = \fint_{-1}^{1} \dfrac{e^{ct}}{t-x}\, dt, \ -1 < x < 1, \ c \in \mathbb{R}.$

A simple calculation yields

$$\begin{aligned} I(x, c) &= e^{cx}[Ei(c(1-x)) + E_1(c(1+x))] && \text{if } c > 0, \\ &= \ln[(1-x)/(1+x)] && \text{if } c = 0, \\ &= -e^{-|c|x}[Ei(|c|(1+x)) + E_1(|c|(1-x))] && \text{if } c < 0, \end{aligned} \tag{8.8}$$

where Ei, E_1 are exponential integrals.

The quadrature rules (8.5) and (8.7) were found to give comparable results in this example. Both, indeed, have similar approximation properties: (8.5) is exact when g is a polynomial of degree $\leqslant 2n-1$, and (8.7) when g is a polynomial of degree $\leqslant 2n$. When n is large, however, and the truncation error near the level of machine precision, (8.5) was observed to produce somewhat more accurate results on account of better stability. Measuring cancellation in the respective quadrature sums by the ratio of the absolutely largest quadrature term and the modulus of the quadrature sum, it was found, for example, that for $n = 40$ and $c = 0.5$ the degree of cancellation is 1–2 orders of magnitude larger in (8.7) than in (8.5).

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