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ORTHOGONAL POLYNOMIALS ON THE SEMICIRCLE*

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In the following we present a summary of some recent work on complex polynomials orthogonal over the unit semicircle with respect to an inner product which is non-Hermitian. The interest in such polynomials was purely intellectual, at first, but took on a more practical bent when it was discovered that they can be usefully employed in numerical quadrature over the semicircle. The location of the zeros in the complex plane also presents questions of intrinsic as well as practical interest.

1. Inner products and related polynomials

Let w be a weight function which is analytic on the unit semidisc $D_+ = \{z \in \boldsymbol{C}\colon |z| < 1, \operatorname{Im} z > 0\}$, nonnegative and $\not\equiv 0$ on $[-1,1]$, and integrable over the boundary $\partial D_+ = \Gamma \cup [-1,1]$. Along with the classical inner product

$$[f, g] = \int_{-1}^{1} f(x)\overline{g(x)}\,w(x)\,dx, \tag{1.1}$$

we consider the complex (non-Hermitian) inner product

$$(f, g) = \int_{\Gamma} f(z)g(z)\frac{w(z)}{iz}\,dz = \int_{0}^{\pi} f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})\,d\theta \tag{1.2}$$

(no conjugation of the second factor!). The (monic) polynomials orthogonal with respect to the inner product in (1.1) will be denoted by $p_r(\cdot) = p_r(\cdot; w)$,

$$[p_k, p_l]\begin{cases} = 0, & k \neq l, \\ > 0, & k = l, \end{cases} \quad k, l = 0, 1, 2, \ldots, \tag{1.3}$$

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those orthogonal with respect to the inner product in (1.2) (if they exist) by $\pi_r(\cdot) = \pi_r(\cdot; w)$,

$$(\pi_k, \pi_l)\begin{cases} = 0, & k \neq l, \\ \neq 0, & k = l, \end{cases} \quad k, l = 0, 1, 2, \ldots \tag{1.4}$$

We remark that (1.4) could not be satisfied if integration in (1.2) were over the full circle ∂D (assuming w analytic in $D = \{z \in C: |z| < 1\}$), since, by Cauchy's theorem, the inner product in (1.4) would then have the value $2\pi \cdot \pi_k(0)\pi_l(0)$.

It is well known that the orthogonal polynomials p_r in (1.3) satisfy a three-term recurrence relation,

$$y_{k+1} = (z - a_k)y_k - b_k y_{k-1}, \quad k = 0, 1, 2, \ldots, \tag{1.5}$$

where $a_k = a_k(w)$ are real and $b_k = b_k(w)$ positive. Indeed, $y_{-1} = 0$, $y_0 = 1$ yields $y_k = p_k(z; w)$. A second (linearly independent) solution of (1.5) is given by the so-called associated polynomials,

$$q_k(z) = q_k(z; w) = \int_{-1}^{1} \frac{p_k(z; w) - p_k(x; w)}{z - x} w(x)\,dx, \quad k = 0, 1, 2, \ldots, \tag{1.6}$$

and is generated by the initial values $y_{-1} = -1$, $y_0 = 0$ (assuming $b_0 = [1, 1]$). We need both, the orthogonal and the associated, polynomials in order to construct the complex polynomials π_r.

2. Existence and representation

In the special case $w(z) \equiv 1$, existence and uniqueness of the orthogonal polynomials $\{\pi_r\}$ was originally proved via moment determinants ([2]). It is now possible to construct the polynomias more elegantly, even for the more general weight functions w considered in Section 1. Indeed, in [3] it is shown that the (monic) polynomials $\pi_r(\cdot) = \pi_r(\cdot; w)$ exist uniquely, assuming only that

$$\operatorname{Re} \mu_0 \neq 0, \quad \mu_0 = \int_0^{\pi} w(e^{i\theta})\,d\theta. \tag{2.1}$$

They can be represented, moreover, in terms of the classical orthogonal polynomials $p_r(\cdot) = p_r(\cdot; w)$ and the associated polynomials $q_r(\cdot) = q_r(\cdot; w)$ (cf. (1.6)) by means of

$$\pi_n(z) = p_n(z) - i\theta_{n-1} p_{n-1}(z), \quad n = 0, 1, 2, \ldots, \tag{2.2}$$

where

$$\theta_{n-1} = \theta_{n-1}(w) = \frac{\mu_0 p_n(0) + i q_n(0)}{i\mu_0 p_{n-1}(0) - q_{n-1}(0)}, \quad n = 0, 1, 2, \ldots \tag{2.3}$$

The condition (2.1) ensures that the constants θ_{n-1} are well defined, i.e., the denominators in (2.3) do not vanish. These constants play a prominent role in the present theory. They can be defined, alternatively, by the nonlinear recursion

$$\theta_n = ia_n + \frac{b_n}{\theta_{n-1}}, \quad n = 0, 1, 2, \ldots; \qquad \theta_{-1} = \mu_0, \tag{2.4}$$

where $a_n = a_n(w)$, $b_n = b_n(w)$ are the recursion coefficients in (1.5).

An easy computation based on (2.2) shows that

$$(\pi_n, \pi_n) = \theta_{n-1}[p_{n-1}, p_{n-1}], \quad n = 1, 2, \ldots; \qquad (\pi_0, \pi_0) = \mu_0. \tag{2.5}$$

EXAMPLE 2.1. *Jacobi weight* $w^{(\alpha,\beta)}(z) = (1-z)^\alpha(1+z)^\beta$, $\alpha > -1$, $\beta > -1$.

One computes $\mu_0 = \pi + i\int_{-1}^{1} w^{(\alpha,\beta)}(x)/x\,dx$, where the integral is a Cauchy principal value integral. Therefore, $\mathrm{Re}\,\mu_0 \neq 0$, and the orthogonal polynomials $\pi_r(\cdot; w^{(\alpha,\beta)})$ exist uniquely.

EXAMPLE 2.2. *Symmetric weight.*

Here, w is assumed analytic in $D = \{z \in \mathbf{C}\colon |z| < 1\}$ and satisfying

$$w(-z) = w(z), \quad z \in D; \qquad w(0) > 0. \tag{2.6}$$

In this case, $\mu_0 = \pi w(0) > 0$, hence the polynomials $\pi_r(\cdot) = \pi_r(\cdot; w)$ again exist uniquely. Moreover, since all coefficients $a_k = a_k(w)$ in (1.5) are zero, it follows from (2.4) that $\theta_n > 0$ for $n \geqslant 0$, hence, by (2.5), that $(\pi_n, \pi_n) > 0$ for $n \geqslant 0$, notwithstanding that π_n is complex-valued.

EXAMPLE 2.3. $w(z) = z^2$.

In this case, clearly, $\mu_0 = \int_0^\pi e^{2i\theta}\,d\theta = 0$, and the polynomials $\pi_r(\cdot; w)$ do not exist, even though the $p_r(\cdot; w)$ do.

3. Recurrence relation

From the property $(zp, q) = (p, zq)$ of the inner product (1.2) it is clear that the polynomials $\{\pi_r(\cdot; w)\}$, if they exist, must satisfy a three-term recurrence relation. We write it in the form

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

where $\alpha_k = \alpha_k(w)$, $\beta_k = \beta_k(w)$, in general, are complex. An elementary computation, based on (2.2) and (1.5), yields the following formulae for these coefficients:

$$\begin{gathered} \alpha_0 = \theta_0 - ia_0; \qquad \alpha_k = \theta_k - \theta_{k-1} - ia_k, \quad k = 1, 2, \ldots; \\ \beta_k = \theta_{k-1}(\theta_{k-1} - ia_{k-1}), \qquad k = 1, 2, \ldots \end{gathered} \tag{3.2}$$

(The coefficient β_0 in (3.1) is not needed, but is conveniently defined by $\beta_0 = \mu_0$.)

For symmetric weight functions (cf. Example 2.2), since $a_k = 0$, it follows that all α_k are real and $\beta_k = \theta_{k-1}^2 > 0$.

Comparison of the coefficient of z^k on the left and right of (3.1) easily yields

$$\pi_n(z;\, w) = z^n - \Big(i\theta_{n-1} + \sum_{m=0}^{n-1} a_m\Big) z^{n-1} + \dots \tag{3.3}$$

This gives useful information about the location of the zeros of π_n (cf. Section 4). Another consequence of (3.1) is the fact that these zeros are the eigenvalues of the matrix

$$J_n(w) = \begin{bmatrix} i\alpha_0 & 1 & & & 0 \\ \beta_1 & i\alpha_1 & 1 & & \\ & \beta_2 & i\alpha_2 & & \\ & & \ddots & & \cdot\, 1 \\ 0 & & & \beta_{n-1} & i\alpha_{n-1} \end{bmatrix}. \tag{3.4}$$

This can be used to compute the zeros, especially in the symmetric case, where the problem can be reduced to an eigenvalue problem for a real, nonsymmetric, tridiagonal matrix [3], § 6.1.

4. Zeros

Relatively complete results are known only for symmetric weight functions (cf. Example 2.2). In this case one knows that all zeros are located in the upper half of the complex plane, symmetrically with respect to the imaginary axis [3], Theorem 6.1, and, in fact, are all contained in the unit upper semidisc D_+, with the possible exception of a (simple) zero iy_0, $y_0 \geqslant 1$ [3], Theorem 6.2. We sketch a proof of this last statement.

According to a result of Giroux [4], either all zeros are in the upper half plane, or all are in the lower half plane. Equation (3.3) (where $\theta_{n-1} > 0$ and all $a_m = 0$) shows that the first alternative must hold. In fact, more precisely [4], if ζ is a zero of $\pi_n(\cdot;\, w)$, then

$$\operatorname{Im}\zeta > 0, \quad |\operatorname{Re}\zeta| \leqslant \xi_n < 1, \tag{4.1}$$

where ξ_n is the largest zero of $p_n(\cdot;\, w)$. It thus suffices to show $|\zeta| < 1$.

Assume first $\operatorname{Re}\zeta \neq 0$, so that by symmetry, ζ and $-\bar\zeta$ are both zeros of π_n and $n \geqslant 2$. Then, by (2.2),

$$\pi_n(x) = p_n(x) - i\theta_{n-1}\, p_{n-1}(x) = (x-\zeta)(x+\bar\zeta)\, r_{n-2}(x), \tag{4.2}$$

where $r_{n-2} \not\equiv 0$ is monic of degree $n-2$. Multiplying (4.2) by $\bar r_{n-2}$ and using the orthogonality of p_n and p_{n-1} to polynomials of lower degree, there follows

$$(4.3)\qquad 0 = \int_{-1}^{1} \pi_n(x)\overline{r_{n-2}(x)}w(x)\,dx = \int_{-1}^{1} (x-\zeta)(x+\bar{\zeta})|r_{n-2}(x)|^2 w(x)\,dx.$$

Noting $(x-\zeta)(x+\bar{\zeta}) = x^2-2ix\,\mathrm{Im}\,\zeta-|\zeta|^2$, and taking the real part of (4.3), yields

$$\int_{-1}^{1} (x^2-|\zeta|^2)|r_{n-2}(x)|^2 w(x)\,dx = 0,$$

which clearly implies $|\zeta| < 1$. In the same way one shows that π_n cannot have two (distinct or confluent) zeros on the imaginary axis with imaginary parts $\geqslant 1$. This completes the proof.

An important example is provided by the Gegenbauer weight

$$(4.4)\qquad w(z) = w^\lambda(z) = (1-z^2)^{\lambda-1/2}, \qquad \lambda > -\frac{1}{2}.$$

Can there be any zero of $\pi_n(\cdot;\, w^\lambda)$ on the imaginary axis outside the unit disc? Suppose $\zeta = iy$, $y \geqslant 1$, is one. Then, by (2.2), since clearly $p_{n-1}(iy) \neq 0$, one finds

$$(4.5)\qquad \omega_n(y) = \theta_{n-1},$$

where $\omega_n(y) = p_n(iy)/(ip_{n-1}(iy))$. From the recurrence formula (1.5) one easily deduces that

$$(4.6)\qquad \omega_1(y) = y; \qquad \omega_k(y) = y+\frac{b_{k-1}}{\omega_{k-1}(y)}, \quad k = 2, 3, \ldots$$

Since $y \geqslant 1$ and $b_{k-1} > 0$, this shows that $\omega_n(y)$ is real and

$$(4.7)\qquad \omega_n(y) \geqslant 1, \quad \text{all } n \geqslant 1.$$

On the other hand, $\theta_{n-1} = \theta_{n-1}(w^\lambda)$ can be expressed explicitly in terms of gamma functions, which, combined with known inequalities for gamma function ratios, yields [3], pp. 401–402,

$$(4.8)\qquad \theta_{n-1} < 1, \quad \text{all } n \geqslant 2.$$

The two inequalities (4.7), (4.8) show that (4.5) is impossible when $n \geqslant 2$. Hence, *all zeros of* $\pi_n(\cdot;\, w^\lambda)$, $n \geqslant 2$, *lie in* D_+. This is also true for $n = 1$, if $\lambda > 0$, but *not* for $n = 1$ and $-\frac{1}{2} < \lambda \leqslant 0$.

Interestingly, the polynomial $\pi_n^\lambda = \pi_n(\cdot;\, w^\lambda)$ satisfies a linear second-order differential eqation,

$$(4.9)\qquad P(z)y''+Q(z)y'+R(z)y = 0,$$

where P, Q and R are cubic, quadratic and linear polynomials in z, respectively [3], § 7. Since all points in D_+ happen to be regular points for (4.9), it follows that the zeros of π_n^λ are simple. Indeed, if there were a multiple zero ζ, it would necessarily have to be in D_+, so that $\pi_n^\lambda(\zeta) = (d/dz)\pi_n^\lambda(\zeta) = 0$ would imply $\pi_n^\lambda \equiv 0$, a contradiction.

There is considerable numerical evidence suggesting that the absence of zeros outside of D_+ (when $n \geq 2$) holds also for the Jacobi weight $w^{(\alpha,\beta)}$ (cf. Example 2.1) for any $\alpha > -1$, $\beta > -1$. Nevertheless, this is not a property valid for general weight functions: In [1] we construct a (symmetric!) weight function w_a (depending on a parameter a) such that $\pi_n(\cdot; w_a)$, for any fixed even n, has a zero iy_0, $y_0 > 1$, provided a is large enough. Indeed, as $a \to \infty$, zeros iy_0 with y_0 arbitrarily large can be so produced. Similarly, another weight function w^a is constructed which has analogous properties for n odd.

5. Applications

If $\pi_n(\cdot; w)$ has n simple (complex) zeros ζ_ν, $\nu = 1, 2, \ldots, n$, one can construct a Gauss–Christoffel quadrature formula for integrals over the semicircle,

$$\tag{5.1} \begin{gathered} \int_0^\pi g(e^{i\theta}) w(e^{i\theta})\, d\theta = \sum_{\nu=1}^n \sigma_\nu g(\zeta_\nu) + R_n(g), \\ R_n(g) = 0, \quad \text{all } g \in \boldsymbol{P}_{2n-1}. \end{gathered}$$

If w is symmetric (cf. Example 2.2), the vector $\sigma^T = [\sigma_1, \sigma_2, \ldots, \sigma_n]$ of the weights in (5.1) can be obtained from a linear system of equations $V_n \sigma = e_1$, where the columns of V_n are eigenvectors of a real, nonsymmetric, tridiagonal matrix (see [2], § 7, for the case $w \equiv 1$) and $e_1^T = [1, 0, \ldots, 0]$ is the first coordinate vector. To a pair of (distinct) zeros $(\zeta_\nu, -\bar{\zeta}_\nu)$ there corresponds a pair $(\sigma_\nu, \bar{\sigma}_\nu)$ of conjugate complex weights, and to a purely imaginary zero ζ_ν a real weight σ_ν.

The example $g(z) = ce^z$, $c > 0$ (and $w \equiv 1$) shows [2], Example 7.1, that the quadrature formula (5.1) can outperform its two closest competitors: the Gauss–Legendre formula (with Gaussian nodes on the semicircle $\{e^{i\theta}\colon 0 < \theta < \pi\}$ and the composite trapezoidal rule.

The formula (5.1) can also be used for integration over the full circle, if the latter is broken up into two halves and the lower half transformed into the upper by a change of variables. In this way, one can numerically implement Cauchy's theorem. To illustrate, suppose we want to approximate the first derivative $f'(a)$ at a real point a, assuming f analytic in the disc $|z-a| \leq h/2$ and mapping reals into reals. Then,

$$\tag{5.2} f'(a) = \frac{1}{\pi h} \int_0^\pi e^{-i\theta} [f(a + \tfrac{1}{2}he^{i\theta}) - f(a - \tfrac{1}{2}he^{i\theta})]\, d\theta,$$

and (5.1) (with $w \equiv 1$) and the symmetry properties mentioned above give

$$\tag{5.3} f'(a) \approx \frac{2}{\pi h} \sum_{\nu=1}^{n/2} \operatorname{Re} \left\{ \frac{\sigma_\nu}{\zeta_\nu} [f(a + \tfrac{1}{2}h\zeta_\nu) - f(a - \tfrac{1}{2}h\zeta_\nu)] \right\}, \qquad n \text{ even}.$$

The error is $O(h^{2n})$ as $h \to 0$.

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