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SOME APPLICATIONS AND NUMERICAL METHODS FOR ORTHOGONAL POLYNOMIALS*

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We restrict ourselves here to polynomials which are orthogonal on the real line relative to a real-valued (often positive) measure. These are the ones best understood, both theoretically and computationally. It should be observed, nevertheless, that polynomials orthogonal on curves and domains in the complex plane, and orthogonal polynomials in several variables, are also of great theoretical and practical interest. Their computational aspects, however, are less well understood and, to a large extent, remain to be studied.

We begin, in Section 1, with defining orthogonal polynomials and introducing notation. In Section 2 we review some classical applications of orthogonal polynomials, including recent extensions. Section 3 is devoted to applications to spline approximation, summation of series and special functions. These well illustrate the need for effective methods of generating nonclassical orthogonal polynomials. Section 4 puts forth the difficulties inherent in constructive methods based on moments. The question of whether "modified moments" improve matters is discussed in Section 5, and a suitable algorithm described in Section 6. Section 7 deals with a more generally applicable, though less economic, algorithm for computing orthogonal polynomials. Finally, in Section 8, we indicate an effective method of generating Gaussian quadrature rules.

1. Orthogonal polynomials

Let $d\sigma$ be a real-valued measure on the real line $\boldsymbol{R}$ (i.e., $\sigma(t)$ a bounded function). The measure is called *positive* if $\sigma(t)$ is nondecreasing. It is called a *discrete* measure [*discrete N-point* measure] if the support $\operatorname{supp}(d\sigma) = \{t\in \boldsymbol{R}\colon\ \sigma(t+\varepsilon) \neq \sigma(t-\varepsilon)$ for all $\varepsilon > 0$ sufficiently small$\}$ is denumerable [con-

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tains exactly N points]. We assume that supp$(d\sigma)$ contains at least N points, $N \leqslant \infty$, and that the *moments*

$$\mu_r = \mu_r(d\sigma) = \int_{\boldsymbol{R}} t^r \, d\sigma(t), \qquad r = 0, 1, \ldots, 2N-1, \tag{1.1}$$

exist. Then on $\boldsymbol{P}_{N-1}$, the set of polynomials of degree $\leqslant N-1$, there is defined a formal inner product (a true inner product, if $d\sigma$ is positive)

$$(p, q)_{d\sigma} = \int_{\boldsymbol{R}} p(t) q(t) \, d\sigma(t), \qquad p, q \in \boldsymbol{P}_{N-1}. \tag{1.2}$$

A sequence of (monic) polynomials

$$\pi_r(t) = t^r + \text{lower-degree terms}, \qquad r = 0, 1, \ldots, N-1, \tag{1.3}$$

is said to be *orthogonal* with respect to the measure $d\sigma$ if

$$(\pi_r, \pi_s)_{d\sigma} \begin{cases} = 0, & r \neq s, \\ \neq 0, & r = s, \end{cases} \quad r, s = 0, 1, \ldots, N-1. \tag{1.4}$$

We write $\pi_r(\cdot) = \pi_r(\cdot; d\sigma)$ if we want to emphasize the measure $d\sigma$ with respect to which π_r is orthogonal.

The sequence of orthogonal polynomials $\{\pi_r(\cdot; d\sigma)\}_{r=0}^{N-1}$ exists uniquely if

$$\det H_n \neq 0, \qquad H_n = \{\mu_{i+j}(d\sigma)\}_{i,j=0}^{n-1}, \qquad n = 1, 2, \ldots, N. \tag{1.5}$$

The conditions (1.5) hold, for example, if $d\sigma$ is positive, in which case indeed $\det H_n > 0$.

Classical examples (with $N = \infty$) are the Legendre and Jacobi polynomials, with absolutely continuous measures $d\sigma(t) = dt$ and $d\sigma(t) = (1-t)^\alpha (1+t)^\beta \, dt$ ($\alpha > -1$, $\beta > -1$), both supported on $[-1, 1]$, the Laguerre polynomials with $d\sigma(t) = t^\alpha e^{-t} \, dt$ on $[0, \infty]$ ($\alpha > -1$), and the Hermite polynomials with $d\sigma(t) = e^{-t^2} dt$ on $[-\infty, \infty]$. Examples of discrete orthogonal polynomials are those of Charlier supported on the nonnegative integers with a Poisson probability distribution, and those of Chebyshev and Krawtchouk supported on $\{0, 1, \ldots, N-1\}$ with a uniform and binomial distribution, respectively.

2. Classical applications

2.1. Least squares approximation and orthogonal expansion. One of the oldest applications, in fact a problem that led to the conception of orthogonal polynomials in the work of Chebyshev [1], is the problem of *least squares approximation*: Given a function f on a set $S \subset \boldsymbol{R}$, find a polynomial of degree n,

$$p_n(t) = \sum_{r=0}^{n} c_r \pi_r(t), \qquad t \in S, \tag{2.1}$$

such that the weighted mean square error

$$\int_{\mathbb{R}} [f(t)-p_n(t)]^2\, d\sigma(t) \tag{2.2}$$

is minimized. Here, $d\sigma$ is a positive measure whose support is S — typically, a discrete set of $N(> n+1)$ points or an interval (finite or infinite). If we choose the polynomials π_r in (2.1) to be those orthogonal in the sense of (1.4), then the solution is well known to be

$$c_r = \frac{(f, \pi_r)_{d\sigma}}{(\pi_r, \pi_r)_{d\sigma}}, \qquad r = 0, 1, 2, \ldots \tag{2.3}$$

These are simply the Fourier coefficients of f with respect to the orthogonal system $\{\pi_r\}$. If the support of $d\sigma$ is infinite, and we let n go to infinity, the approximation (2.1), (2.3) becomes an *orthogonal expansion*,

$$f(t) \sim \sum_{r=0}^{\infty} c_r \pi_r(t), \tag{2.4}$$

for which there is a vast body of literature; see, e.g., Szegö [27], Ch. 9, Freud [3], Ch. 4, Suetin [26] and Rusev [22].

Computationally, (2.3) requires numerical integration — most naturally Gaussian quadrature (cf. Section 2.2) — unless $d\sigma$ is a finite discrete measure. In either case, rewriting (2.3) in the form

$$c_0 = \frac{(f, \pi_0)_{d\sigma}}{(\pi_0, \pi_0)_{d\sigma}}, \qquad c_r = \frac{(f - \sum_{s=0}^{r-1} c_s \pi_s, \pi_r)_{d\sigma}}{(\pi_r, \pi_r)_{d\sigma}}, \qquad r = 1, 2, 3, \ldots, \tag{2.3'}$$

will be advantageous, as it helps preserving accuracy in the presence of rounding errors (Conte and de Boor [2], pp. 264–265).

Least squares approximation may be combined with interpolation at given points $t = \zeta_j$, $j = 1, 2, \ldots, m$: Find a polynomial $p_{n,m} \in \boldsymbol{P}_{m+n}$ such that

$$\int_{\mathbb{R}} [f(t) - p_{n,m}(t)]^2\, d\sigma(t) = \min \tag{2.5}$$

subject to

$$p_{n,m}(\zeta_j) = f(\zeta_j), \qquad j = 1, 2, \ldots, m. \tag{2.6}$$

Writing

$$p_{n,m}(t) = p_m(f; t) + \psi_m(t) \sum_{r=0}^{n} c_r \pi_r(t), \tag{2.7}$$

where $p_m(f;\cdot)$ is the polynomial of degree $m-1$ interpolating f at the ζ_j's and $\psi_m(t) = \prod_{j=1}^{m} (t - \zeta_j)$, the problem (2.5), (2.6) assumes the form

$$\int_{\mathbb{R}} \left[\frac{f(t) - p_m(f; t)}{\psi_m(t)} - \sum_{r=0}^{n} c_r \pi_r(t)\right]^2 \psi_m^2(t)\, d\sigma(t) = \min. \tag{2.8}$$

This shows that the constrained problem (2.5), (2.6) amounts to an "ordinary" least squares problem, but for the new function $\bar{f}(t) = [f(t) - p_m(f;t)]/\psi_m(t)$ and with a new measure $d\bar{\sigma}(t) = \psi_m^2(t)\,d\sigma(t)$; cf. Gautschi and Lin [17]. There arises the interesting computational problem of generating $\pi_r(\cdot; d\bar{\sigma})$, knowing $\pi_r(\cdot; d\sigma)$. Similarly, if one tries to combine least squares approximation by rationals with matching of poles η_k outside the support of $d\sigma$, one is led to considering the analogous problem with $d\bar{\sigma}(t) = d\sigma(t)/\omega_m^2(t)$, where $\omega_m(t) = \prod_{k=1}^{m}(t-\eta_k)$.

2.2. Numerical quadrature. With the measure $d\sigma$ (see Section 1) we may associate for each $n \leqslant N$ the *Gaussian quadrature* formula

$$\int_{\boldsymbol{R}} f(t)\,d\sigma(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f) \tag{2.9}$$

having the property that $R_n(f) = 0$ for all $f \in \boldsymbol{P}_{2n-1}$. If $d\sigma$ is positive, the formula exists uniquely and has maximum degree of exactness. The nodes $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$ are indeed the zeros of $\pi_n(\cdot; d\sigma)$ and all weights $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$ – called *Christoffel numbers* – are positive. Their computation is discussed in Section 8.

An interesting extension of (2.9) is the so-called *Gauss–Kronrod quadrature* formula

$$\int_{\boldsymbol{R}} f(t)\,d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n^*(f), \tag{2.10}$$

where the nodes τ_ν are the same as in (2.9), but new nodes $\tau_\mu^* = \tau_\mu^{(n)*}(d\sigma)$ and new weights $\sigma_\nu = \sigma_\nu^{(n)}(d\sigma)$, $\sigma_\mu^* = \sigma_\mu^{(n)*}(d\sigma)$ are introduced and selected so as to give (2.10) maximum degree of exactness, that is, $R_n^*(f) = 0$ for all $f \in \boldsymbol{P}_{3n+1}$ (at least). It turns out that the nodes τ_μ^* must be the zeros of the polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; d\sigma)$ of degree $n+1$ satisfying the orthogonality condition

$$\int_{\boldsymbol{R}} \pi_{n+1}^*(t)\,p(t)\,d\sigma^*(t) = 0, \quad \text{all } p \in \boldsymbol{P}_n, \tag{2.11}$$

where $d\sigma^*(t) = \pi_n(t; d\sigma)\,d\sigma(t)$ is a measure that changes sign n times on its support (if $d\sigma$ is positive). As a result, the reality of the nodes τ_μ^* is no longer assured, but can be proved for special classes of measures, for example, the Gegenbauer measure $d\sigma(t) = (1-t^2)^{\lambda - 1/2}\,dt$ on $[-1, 1]$ for $0 \leqslant \lambda \leqslant 2$, or the "Geronimus measure" $d\sigma(t) = (1-t^2)^{1/2}\,dt/(1-\mu t^2)$ for $-\infty < \mu \leqslant 1$. Not only are the nodes τ_μ^* real in these cases, but they are all contained in $[-1, 1]$ and interlace with the nodes τ_ν. Moreover, all weights σ_ν, σ_μ^* in (2.10) are positive (if $0 \leqslant \lambda \leqslant 1$ in the Gegenbauer case). See [14] for a survey of Gauss–Kronrod quadrature and related matters. Other interesting quadrature formulae, leading to still other types of orthogonality, are those of maximum degree of exactness involving multiple nodes. They were studied first by Turán and subsequently by Chakalov, Popoviciu, Stancu and others; see, e.g., Gautschi [6], § 2.2.

2.3. Padé approximation. The theory of Padé approximation is closely tied up with orthogonal polynomials and Gaussian quadrature if one deals with formal power series

$$f(z) = \mu_0 + \mu_1 z + \mu_2 z^2 + \ldots \tag{2.12}$$

in which the coefficients are moments (cf. (1.1)) of some given (positive) measure $d\sigma$. The $[m,n]$-Padé approximant $f[m,n](z)$ — a rational function of type $[m,n]$ having maximum "contact" with f at $z=0$ — is then given, for $m = n-1$, by

$$f[n-1, n](z) = \sum_{\nu=1}^{n} \frac{\lambda_\nu}{1-\tau_\nu z}, \qquad n = 1, 2, 3, \ldots, \tag{2.13}$$

where $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$, $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$ are the weights and nodes of the Gaussian quadrature formula for $d\sigma$ (cf. (2.9)), and for $m > n$ by

$$f[n-1+j, n](z) = \mu_0 + \ldots + \mu_{j-1} z^{j-1} + z^j \sum_{\nu=1}^{n} \frac{\lambda_{\nu j}}{1-\tau_{\nu j} z}, \tag{2.14}$$
$$n = 1, 2, 3, \ldots, \; j \text{ even},$$

where $\lambda_{\nu j} = \lambda_\nu^{(n)}(d\sigma_j)$, $\tau_{\nu j} = \tau_\nu^{(n)}(d\sigma_j)$ are the weights and nodes of the Gauss formula for $d\sigma_j(t) = t^j d\sigma(t)$. If j is even, as assumed in (2.14), $d\sigma_j$ is positive and the orthogonal polynomial $\pi_n(\cdot; d\sigma_j)$ exists. If j is odd, this may no longer be true, but if it is, and $\pi_n(\cdot; d\sigma_j)$ has simple zeros, (2.14) continues to hold.

3. Other applications

The applications described in this section are of more recent origin.

3.1. Moment-preserving spline approximation. For simplicity, we consider only the problem on an infinite half line: Given a function f on $[0, \infty]$, vanishing sufficiently rapidly at infinity, find a spline function of degree m,

$$s_{n,m}(t) = \sum_{\nu=1}^{n} a_\nu (\tau_\nu - t)_+^m, \qquad 0 \leqslant t < \infty, \tag{3.1}$$

with knots

$$\tau_1 > \tau_2 > \ldots > \tau_n > 0, \tag{3.2}$$

such that its first $2n$ moments agree with those of f,

$$\int_0^\infty t^j s_{n,m}(t)\,dt = \int_0^\infty t^j f(t)\,dt, \qquad j = 0, 1, \ldots, 2n-1. \tag{3.3}$$

In (3.1), the plus sign is the cutoff symbol: $x_+ = x$ if $x > 0$ and $x_+ = 0$ if $x \leqslant 0$. The (real) coefficients a_ν and knots τ_ν are all unknown and to be determined. We may think of (3.3) as being a finite moment problem where the solution is required to be a spline of type (3.1), (3.2).

If $f \in C^{m+1}[0,\infty]$ and is such that the integrals on the right of (3.3) exist and $\lim_{t\to\infty} t^{2n+\mu} f^{(\mu)}(t) = 0$ for $\mu = 0, 1, \ldots, m$, then the solution (Gautschi [9], Gautschi and Milovanović [16]) can be shown to be $\tau_\nu = \tau_\nu^{(n)}(d\sigma_m)$ and $a_\nu = \tau_\nu^{-(m+1)} \lambda_\nu^{(n)}(d\sigma_m)$, where

$$d\sigma_m(t) = \frac{(-1)^{m+1}}{m!} t^{m+1} f^{(m+1)}(t)\, dt \quad \text{on } [0,\infty], \tag{3.4}$$

provided the measure (3.4) admits an n-point Gaussian quadrature formula (cf. (2.9)) with distinct positive nodes. The error, then, is given, for any $r > 0$, by

$$f(r) - s_{n,m}(r) = R_n(g_r; d\sigma_m), \qquad g_r(t) = t^{-(m+1)}(t-r)_+^m, \tag{3.5}$$

where $R_n(g; d\sigma_m)$ is the remainder term of the Gauss formula when applied to the function g. Note that $d\sigma_m$, in general, is not a positive measure, but is so, for every $m \geqslant 0$, if f is completely monotonic on $[0,\infty]$.

If one only assumes the existence of the moments on the right of (3.3), but no further smoothness, an analogous solution can be given in terms of Gauss quadrature relative to a certain moment functional [16], Thm. 2.1. The case of a finite interval is a bit more involved and is treated in [4].

3.2. Summation of series (Gautschi and Milovanović [15]). Series such as

$$\sum_{k=1}^{\infty} (-1)^{k-1} F(k), \tag{3.6}$$

involving the Laplace transform

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt, \qquad \operatorname{Re} s > 0, \tag{3.7}$$

are apt to converge slowly on account of Watson's lemma, which, typically, implies $F(k) \sim k^{-1}$ as $k \to \infty$. If the "original" function f is known and smooth, however, then the series (3.6) can be summed very effectively by Gaussian quadrature with respect to the measure

$$d\sigma(t) = \frac{dt}{e^t + 1} \quad \text{on } [0,\infty]. \tag{3.8}$$

Indeed, it suffices to apply this quadrature rule to the right-hand side of

$$\sum_{k=1}^{\infty} (-1)^{k-1} F(k) = \int_0^\infty f(t) \frac{dt}{e^t + 1}. \tag{3.9}$$

The measure here is nonclassical and requires methods such as those in Section 6 to generate the respective orthogonal polynomials. Similar methods apply to the series $-\sum_{k=1}^{\infty} F'(k)$ and $-\sum_{k=1}^{\infty} (-1)^{k-1} F'(k)$, where the relevant measures are $d\sigma(t) = t\, dt/(e^t - 1)$ and $d\sigma(t) = t\, dt/(e^t + 1)$, respectively.

To give a numerical example, consider $F(s) = s^{-1}e^{-1/s}$. In this case, $f(t) = J_0(2\sqrt{t})$ (J_0 = Bessel function of order zero) and

$$\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} e^{-1/k} = \int_0^{\infty} J_0(2\sqrt{t}) \frac{dt}{e^t+1} = .1971079\ldots \tag{3.10}$$

Applying the n-point Gauss formula (with $d\sigma(t) = dt/(e^t+1)$) to the integral in (3.10) yields approximations to the sum having relative errors 1.8×10^{-2}, 9.7×10^{-7}, 1.1×10^{-17} for $n = 2$, 4 and 8, respectively.

3.3. Computation of inhomogeneous Airy functions. The inhomogeneous Airy functions $\mathrm{Gi}(x)$ and $\mathrm{Hi}(x)$ are solutions of the differential equation

$$\frac{dy^2}{dx^2} - xy = \begin{cases} -\dfrac{1}{\pi} & \text{for } \mathrm{Gi}(x), \\ \dfrac{1}{\pi} & \text{for } \mathrm{Hi}(x) \end{cases} \tag{3.11}$$

satisfying certain initial conditions at $x = 0$. They occur in Raman scattering, harmonic oscillator models for large quantum numbers, and elsewhere. Known integral representations (Lee [20]),

$$\begin{aligned} \mathrm{Hi}(x) &= \frac{1}{\pi} \int_0^{\infty} \exp(-\tfrac{1}{3}t^3 + tx)\, dt, \\ \mathrm{Gi}(x) &= -\frac{1}{\pi} \int_0^{\infty} \exp(-\tfrac{1}{3}t^3 - \tfrac{1}{2}tx) \cos(\tfrac{1}{2}\sqrt{3}\, tx + \tfrac{2}{3}\pi)\, dt, \end{aligned} \tag{3.12}$$

suggest the application of Gaussian quadrature with measure $d\sigma(t) = \exp(-\frac{1}{3}t^3)\,dt$ on $[0, \infty]$ — once again, a nonclassical measure. The pitfalls inherent in computing orthogonal polynomials for this measure, using moments, are brought home in [8].

4. The difficulty with moments

To put the discussion of constructive methods into proper perspective, it is necessary to recall what is wrong with the classical approach — computing orthogonal polynomials and related quantities from the moments $\mu_r(d\sigma)$ (cf. (1.1)) of the given (positive) measure $d\sigma$. The quantities desired, indeed, are inherently sensitive to small perturbations in the moments.

This is best illustrated in the case of Gaussian quadrature rules. The nodes $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$ and weights $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$ of the n-point formula (cf. (2.9)) are well-defined functions of the first $2n$ moments $\mu_r = \mu_r(d\sigma)$, $r = 0, 1, \ldots, 2n-1$. If we collect them in a vector $[\tau, \lambda] \in \mathbf{R}^{2n}$, where τ and λ are the n-vectors with components τ_ν and λ_ν, and if we denote by $\mu = \mu(d\sigma)$ the $2n$-vector of moments, then the problem of computing the n-point Gauss formula amounts to carrying out the nonlinear map

(4.1) $$G_n\colon R^{2n} \to R^{2n}, \qquad \mu \to \begin{bmatrix} \tau \\ \lambda \end{bmatrix}.$$

The difficulty is that the map G_n becomes rapidly ill-conditioned as n increases, that is, small changes in μ give rise to large changes in $[\tau, \lambda]$, more so the larger n.

To cite a specific result (Gautschi [5]), suppose $d\sigma$ is supported on $[0, 1]$ and normalized so that $\mu_0(d\sigma) = 1$. Then the condition number of G_n (suitably defined) satisfies

(4.2) $$(\operatorname{cond} G_n)(\mu) \geqslant \frac{1}{2} \max_{1 \leqslant \nu \leqslant 1} \left[\frac{\pi_n(-1)}{\cdot \pi_n'(\tau_\nu)} \right]^2,$$

where $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$ and $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$, $\nu = 1, 2, \ldots, n$. The lower bound in (4.2), at least for measures in the Szegö class ([27], Ch. 12), must be expected to grow at an exponential rate somewhat like $n^{-2}(3+\sqrt{8})^{2n}$ as $n \to \infty$. Thus, whatever method is going to be used to implement the map G_n, the presence of rounding errors will soon distort the results beyond recognition.

5. Modified moments

It has been suggested [23] that using *modified moments*

(5.1) $$m_k = m_k(d\sigma) = \int_R p_k(t)\, d\sigma(t), \qquad k = 0, 1, 2, \ldots,$$

in place of the ordinary moments (1.1), where $\{p_k\}$ is a suitable system of polynomials with $\deg p_k = k$, $k = 0, 1, 2, \ldots$, might improve the numerical condition of the map (4.1). The matter has been analyzed in [7], § 3.3, [12] (see also [11], § 5.3), and we briefly state the major conclusions.

We assume the polynomials p_k defining the modified moments to be themselves orthogonal polynomials, orthogonal with respect to a (classical) measure ds that can be chosen at one's convenience. The results, then, assume a simpler form if the modified moments are normalized by

(5.2) $$\tilde{m}_k = d_k^{-1} m_k, \qquad d_k^2 = \int_R p_k^2(t)\, ds(t),$$

and thus made independent of the particular normalization of the polynomials p_k. If the corresponding map is denoted by $\tilde{G}_n$,

(5.3) $$\tilde{G}\colon R^{2n} \to R^{2n}, \qquad \tilde{m} \to \begin{bmatrix} \tau \\ \lambda \end{bmatrix},$$

and if it is meaningful to measure perturbations in terms of absolute errors, then the sensitivity of the map $\tilde{G}_n$ is characterized by the magnitude of its Fréchet derivative $\tilde{G}_n'(\tilde{m}) = (D\tilde{G}_n)(\tilde{m})$. Using the Frobenius norm $\|\cdot\|_F$ to measure the magnitude of linear operators, one then proves that ([7], § 3.3)

$$\|\tilde{G}_n'(\tilde{m})\|_F^2 = \int_{\mathbf{R}} g_n(t; d\sigma)\, ds(t), \tag{5.4}$$

where

$$g_n(t; d\sigma) = \sum_{\nu=1}^{n} \left[h_\nu^2(t) + \frac{1}{\lambda_\nu^2} k_\nu^2(t) \right] \tag{5.5}$$

and h_ν, k_ν are the elementary Hermite interpolation polynomials of degree $2n-1$ defined by

$$\begin{array}{ll} h_\nu(\tau_\mu) = \delta_{\nu\mu}, & h_\nu'(\tau_\mu) = 0, \\ k_\nu(\tau_\mu) = 0, & k_\nu'(\tau_\mu) = \delta_{\nu\mu}, \end{array} \quad \nu, \mu = 1, 2, \ldots, n. \tag{5.6}$$

(Here, $\tau_\mu = \tau_\mu^{(n)}(d\sigma)$ are the Gaussian nodes for the measure $d\sigma$ and $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$ in (5.5) the corresponding Christoffel numbers; $\delta_{\nu\mu}$ denotes the Kronecker symbol.) Therefore, the magnitude of $\tilde{G}_n'(\tilde{m})$, and with it the sensitivity of the map (5.3), depends crucially on the magnitude of the polynomial $g_n(\cdot) = g_n(\cdot; d\sigma)$ in (5.5) on the support of ds. The properties

$$g_n(\tau_\nu) = 1, \quad g_n'(\tau_\nu) = 0, \quad \nu = 1, 2, \ldots, n, \tag{5.7}$$

which easily follow from (5.6), lend credence to the expectation that g_n remains "small", perhaps even smaller than 1. Unfortunately, this is not always the case. We give two examples. (More can be found in [11], § 5.5.)

EXAMPLE 1. *Chebyshev and Jacobi measures.*
In the case of the Chebyshev measure $d\sigma(t) = (1-t^2)^{-1/2}\,dt$ on $[-1,1]$ there is strong numerical evidence suggesting that $g_n(t; d\sigma) \leqslant 1$ on $[-1,1]$ for all $n \geqslant 2$. This would imply $\|\tilde{G}_n'(\tilde{m})\|_F \leqslant \int_{\mathbf{R}} ds(t) = \mu_0(ds)$ for all $n \geqslant 2$, if $\operatorname{supp}(ds) \subseteq [-1,1]$, that is, uniform boundedness of the Fréchet derivative of $\tilde{G}_n$. The same is conjectured, for $n \geqslant 2$, in the case of Jacobi measures $d\sigma(t) = (1-t)^\alpha (1+t)^\beta\, dt$, $-1 < \alpha \leqslant \alpha_0$, $-1 < \beta \leqslant \alpha_0$, where $\alpha_0 = -.3369\ldots$ (see [13]). As the parameter α, or β, gets larger, however, the maximum of g_n on $[-1,1]$, particularly for n large, grows significantly ([12]), causing potential ill-conditioning of the map $\tilde{G}_n$.

EXAMPLE 2. *A doubly supported measure.*
The measure

$$d\sigma(t) = \begin{cases} |t|(1-t^2)^{-1/2}(t^2-\omega^2)^{-1/2}\,dt, & \omega < |t| < 1, \\ 0, & |t| < \omega, \end{cases} \quad 0 < \omega < 1, \tag{5.8}$$

comes up in the study of a diatomic linear chain model [29] (see also [10]). All nodes $\tau_\nu^{(n)}(d\sigma)$, here, are located in the two support intervals $-1 < t < -\omega$ and $\omega < t < 1$, except for one (at the origin) if n is odd. As a consequence, one observes that $g_n(\cdot; d\sigma)$ remains $\leqslant 1$ on the two intervals, but shoots up to a very large value on the "hole" between them. For example, if $n = 40$ and $\omega = 1/3$, the maximum of g_n on $[-\omega, \omega]$ is of the order 10^{20}! Whether or not this gives rise to a large Fréchet derivative in (5.4) depends on the measure ds. If one takes $ds(t) = (1-t^2)^{-1/2}\,dt$ on $[-1, 1]$, then indeed $\|\tilde{G}_n'\|_F \sim 10^9$. If, on the other hand, ds is supported on the same intervals as $d\sigma$, then $\|\tilde{G}_n'\|_F$ remains uniformly bounded.

6. A modified moment algorithm

We now show how the first n coefficients $\alpha_k = \alpha_k(d\sigma)$, $\beta_k = \beta_k(d\sigma)$, $k = 0, 1, \ldots, n-1$, in the recurrence formula

$$\begin{gathered} \pi_{k+1}(t) = (t-\alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \qquad k = 0, 1, \ldots, n-1, \\ \pi_{-1}(t) = 0, \qquad \pi_0(t) = 1 \end{gathered} \tag{6.1}$$

satisfied by the polynomials $\{\pi_r(\cdot; d\sigma)\}$ can be computed from the first $2n$ modified moments $m_k(d\sigma)$, $k = 0, 1, \ldots, 2n-1$, in (5.1). Once these coefficients have been obtained, the Gauss quadrature rule, i.e., the quantities $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$, $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$ in (2.9), can be computed as described in Section 8.

We assume that the polynomials p_k defining the modified moments (5.1) satisfy themselves a recurrence relation like (6.1),

$$\begin{gathered} p_{k+1}(t) = (t-a_k)p_k(t) - b_k p_{k-1}(t), \qquad k = 0, 1, \ldots, n-1, \\ p_{-1}(t) = 0, \qquad p_0(t) = 1, \end{gathered} \tag{6.2}$$

but with coefficients a_k, b_k that are known. (This is the case for $p_k(\cdot) = \pi_k(\cdot; ds)$ when ds is one of the classical measures; ordinary moments are also included with the choice $a_k = b_k = 0$.)

With "mixed moments" $\sigma_{k,l}$ defined by

$$\sigma_{k,l} = \int_{\mathbb{R}} \pi_k(t; d\sigma)\, p_l(t)\, d\sigma(t), \qquad l \geqslant k \geqslant 0 \tag{6.3}$$

(clearly, $\sigma_{k,l} = 0$ for $l < k$), the algorithm in question is initialized by

$$\begin{gathered} \sigma_{-1,l} = 0, \qquad l = 1, 2, \ldots, 2n-2, \\ \sigma_{0,l} = m_l, \qquad l = 0, 1, \ldots, 2n-1, \\ \alpha_0 = a_0 + \frac{m_1}{m_0}, \qquad \beta_0 = m_0, \end{gathered} \tag{6.4$_0$}$$

and continued, for $k = 1, 2, \ldots, n-1$, by

$$
\begin{aligned}
&\sigma_{k,l} = \sigma_{k-1,l+1} - (\alpha_{k-1} - a_l)\sigma_{k-1,l} - \beta_{k-1}\sigma_{k-2,l} + b_l \sigma_{k-1,l-1}, \\
(6.4_k) \qquad & \qquad\qquad\qquad\qquad\qquad\qquad l = k, k+1, \ldots, 2n-k-1, \\
&\alpha_k = a_k + \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \qquad \beta_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}.
\end{aligned}
$$

The first set of relations in (6.4_k) generates a new "row" of mixed moments, using a "five-point computing star", the first two of which, together with the first two of the preceding row, then being used to compute the next coefficients α_k, β_k. The complexity of the algorithm is clearly $O(n^2)$.

The algorithm (6.4), in the case of ordinary moments ($a_k = b_k = 0$) and for discrete measures $d\sigma$, was already proposed by Chebyshev [1]. It was rediscovered, in a slightly different form, by Sack and Donovan [23], and in the form (6.4) by Wheeler [28].

7. A "bootstrap" algorithm

The recursion coefficients α_k, β_k in (6.1) can be represented in terms of the inner product $(\cdot,\cdot)_{d\sigma}$ (cf. (1.2)) by

$$
(7.1) \qquad
\begin{aligned}
\alpha_k(d\sigma) &= \frac{(t\pi_k, \pi_k)_{d\sigma}}{(\pi_k, \pi_k)_{d\sigma}}, \qquad k = 0, 1, 2, \ldots, \\
\beta_k(d\sigma) &= \frac{(\pi_k, \pi_k)_{d\sigma}}{(\pi_{k-1}, \pi_{k-1})_{d\sigma}}, \qquad k = 1, 2, \ldots,
\end{aligned}
$$

where $\pi_r(\cdot) = \pi_r(\cdot; d\sigma)$. Since $\pi_0 = 1$, we can compute α_0 by (7.1) for $k = 0$. This in turn yields π_1, by (6.1) for $k = 0$. Therefore, (7.1) can be used with $k = 1$ to obtain α_1, β_1, whereupon (6.1) for $k = 1$ yields π_2, etc. In this way, alternating between (7.1) and (6.1), we can build up as many coefficients α_k, β_k as are desired. The idea of such an algorithm goes back to Stieltjes [25].

The implementation of this idea is relatively straightforward when $d\sigma$ is a finite discrete measure, since the inner products in (7.1) then involve only finite summations, no integration. For continuous measures $d\sigma$ one can try to approximate the inner product $(\cdot,\cdot)_{d\sigma}$ by a discrete N-point inner product $(\cdot,\cdot)_{d\sigma_N}$ in such a way that $\lim_{N\to\infty}(p, q)_{d\sigma_N} = (p, q)_{d\sigma}$ whenever p, q are polynomials. (For details of how such a discretization may be accomplished, we refer to [5], [7], § 2.2.) Applying the algorithm described above in its discrete version (with measure $d\sigma_N$ for N sufficiently large) then produces approximations to the recursion coefficients α_k, β_k which converge to the true values as $N \to \infty$.

8. Computation of Gaussian quadrature formulae

The recursion coefficients $\alpha_k = \alpha_k(d\sigma)$, $\beta_k = \beta_k(d\sigma)$ in (6.1) define a (in general) infinite *Jacobi matrix*

$$J(d\sigma) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \sqrt{\beta_3} & \\ & & \ddots & \ddots & \ddots \end{bmatrix}. \tag{8.1}$$

Let $J_n = J_{[n\times n]}$ denote the leading $n\times n$ submatrix of J. Then the Gaussian nodes $\tau_\nu = \tau_\nu^{(n)}(d\sigma)$ (cf. (2.9)) are the eigenvalues of J_n and the weights $\lambda_\nu = \lambda_\nu^{(n)}(d\sigma)$ are given by $\lambda_\nu = \mu_0 u_{\nu,1}^2$, where $\mu_0 = \mu_0(d\sigma)$ is the first moment of $d\sigma$ and $u_{\nu,1}$ the first component of the normalized eigenvector u_ν corresponding to the eigenvalue τ_ν (see, e.g., [30], Ch. 2, Exercise 9, or [19]). The problem of computing Gaussian quadrature rules, once the recursion coefficients α_k, β_k are known, thus amounts to solving an eigensystem problem for a symmetric tridiagonal matrix. For this, there are efficient algorithms, for example the QR algorithm (Golub and Welsch [18], Parlett [21], Ch. 8) and reliable software (Smith et al. [24]).

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