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ORTHOGONAL POLYNOMIALS AND QUADRATURE*

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Abstract. Various concepts of orthogonality on the real line are reviewed that arise in connection with quadrature rules. Orthogonality relative to a positive measure and Gauss-type quadrature rules are classical. More recent types of orthogonality include orthogonality relative to a sign-variable measure, which arises in connection with Gauss-Kronrod quadrature, and power (or implicit) orthogonality encountered in Turán-type quadratures. Relevant questions of numerical computation are also considered.

Key words. orthogonal polynomials, Gauss-Lobatto, Gauss-Kronrod, and Gauss-Turán rules, computation of Gauss-type quadrature rules.

AMS subject classifications. 33C45, 65D32, 65F15.

1. Introduction. Orthogonality concepts arise naturally in connection with numerical quadrature, when one tries to optimize the degree of precision. The classical example is the Gaussian quadrature rule, which maximizes the (polynomial) degree of exactness. Closely related quadrature rules are those of Radau and Lobatto, where one or two nodes are prescribed. In Gauss-Kronrod rules about half of the nodes are prescribed, all within the support of the integration measure, which gives rise to orthogonality relative to a sign-variable measure. Quadrature rules with multiple nodes lead naturally to power (or implicit) orthogonality. The classical example here is the Turán quadrature rule.

In the following, these interrelations between orthogonal polynomials and quadrature rules, as well as relevant computational algorithms, are discussed in more detail.

2. Quadrature rules and orthogonality. We begin with the simplest kind of quadrature rule,

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n(f), \tag{2.1}$$

where the integral of a function f relative to some (in general positive) measure $d\lambda$ is approximated by a finite sum involving n values of f at suitably selected distinct nodes τ_ν. The respective error is $R_n(f)$. The support of the measure is usually a finite interval, a half-infinite interval, or the whole real line $\mathbb{R}$, but could also be a finite or infinite collection of mutually distinct intervals or points.

The formula (2.1) is said to have polynomial degree of exactness d if

$$R_n(f) = 0 \quad \text{for all } f \in \mathbb{P}_d, \tag{2.2}$$

where $\mathbb{P}_d$ denotes the set of polynomials of degree $\le d$. Interpolatory formulae (or Newton-Cotes formulae) are those having degree $d = n - 1$. They are precisely the quadrature rules obtained by replacing f in (2.1) by its Lagrange polynomial of degree $\le n-1$ interpolating f at the nodes τ_ν. We denote by

$$\omega_n(t) = \prod_{\nu=1}^{n} (t - \tau_\nu) \tag{2.3}$$

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the node polynomial associated with the rule (2.1), i.e., the monic polynomial of degree n having the nodes τ_ν as its zeros.

We see that, given the n nodes τ_ν, we can always achieve degree of exactness $n-1$. A natural question is how to select the nodes τ_ν and weights λ_ν to do better. This is answered by the following theorem.

THEOREM 2.1. *The quadrature rule* (2.1) *has degree of exactness* $d = n-1+k$, $k \geq 0$, *if and only if both of the following conditions are satisfied:*

(a) *the formula* (2.1) *is interpolatory;*

(b) *the node polynomial* ω_n *satisfies*

$$\int_{\mathbb{R}} \omega_n(t)p(t)d\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{k-1}. \tag{2.4}$$

It is difficult to trace the origin of this theorem, but Jacobi [11] must have been aware of it.

We remark that $k = 0$ corresponds to the Newton-Cotes formula, which requires no condition other than being interpolatory. The requirement (2.4), accordingly, is empty. If $k > 0$, the condition (2.4) is a condition that involves only the nodes τ_ν of (2.1); it imposes exactly k nonlinear constraints on them, in fact, orthogonality (relative to the measure $d\lambda$) of the node polynomial ω_n to the space of all polynomials of degree $\leq k-1$. Once a set of nodes τ_ν has been determined that satisfies this constraint, the condition (a) then uniquely determines the weights λ_ν in (2.1), for example, as the solution of the linear (Vandermonde) system of equations $\sum_{\nu=1}^n \lambda_\nu \tau_\nu^\mu = \int_{\mathbb{R}} t^\mu d\lambda(t)$, $\mu = 0, 1, \ldots, n-1$.

2.1. The Gaussian quadrature rule. If the measure $d\lambda$ is positive, then $k \leq n$, since otherwise (2.4) would have to hold for $k = n+1$, implying that ω_n is orthogonal to all polynomials of degree $\leq n$, hence, in particular, orthogonal to itself, which is impossible. Thus, $k = n$ is optimal, in which case ω_n is orthogonal to all polynomials of lower degree, i.e., ω_n is the (monic) orthogonal polynomial of degree n relative to the measure $d\lambda$. We express this by writing

$$\omega_n(t) = \pi_n(t; d\lambda). \tag{2.5}$$

The interpolatory quadrature rule

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^n \lambda_\nu^G f(\tau_\nu^G) + R_n^G(f) \tag{2.6}$$

corresponding to this node polynomial is precisely the Gaussian quadrature rule for the measure $d\lambda$. It was discovered by Gauss in 1814 ([4]) in the special case of the Lebesgue measure $d\lambda(t) = dt$ on $[-1, 1]$. For general $d\lambda$, its nodes are the zeros of the orthogonal polynomial $\pi_n(\,\cdot\,; d\lambda)$, and its weights λ_ν, the so-called Christoffel numbers, are obtainable by interpolation as above. (See, however, Theorem 3.1 below.)

2.2. The Gauss-Radau quadrature rule. If the support of $d\lambda$ is bounded from one side, say from the left, it is sometimes convenient to take $a = \inf \operatorname{supp} d\lambda$ as one of the nodes, say $\tau_1 = a$. According to Theorem 2.1, this reduces the degree of freedom by one, and the maximum possible value of k is $k = n-1$. If we write $\omega_n(t) = \omega_{n-1}(t)(t-a)$, the polynomial ω_{n-1} having the remaining nodes as its zeros must be orthogonal to all lower-degree polynomials relative to the measure $d\lambda_a(t) = (t-a)d\lambda(t)$, i.e.,

$$\omega_{n-1}(t) = \pi_{n-1}(t; d\lambda_a). \tag{2.7}$$

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The corresponding interpolatory quadrature rule,

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \lambda_1^R f(a) + \sum_{\nu=2}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_n^R(f), \tag{2.8}$$

is called the Gauss-Radau rule for $d\lambda$ (Radau [19]).

There is an analogous rule in the case $b = \sup \operatorname{supp} d\lambda < \infty$, with, say, $\tau_n = b$. Indeed, both rules make sense also in the case $a < \inf \operatorname{supp} d\lambda$ resp. $b > \sup \operatorname{supp} d\lambda$. They are special cases of a quadrature rule already considered by Christoffel in 1858 ([3]).

2.3. The Gauss-Lobatto quadrature rule. If the support of $d\lambda$ is bounded from both sides, we may take $\tau_1 = a \leq \inf \operatorname{supp} d\lambda$ and $\tau_n = b \geq \sup \operatorname{supp} d\lambda$, thereby restricting the degree of freedom once more. The optimal quadrature rule becomes the Gauss-Lobatto rule for $d\lambda$ ([15]),

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \lambda_1^L f(a) + \sum_{\nu=2}^{n-1} \lambda_\nu^L f(\tau_\nu^L) + \lambda_n^L f(b) + R_n^L(f), \tag{2.9}$$

whose interior nodes τ_ν are the zeros of

$$\pi_{n-2}(\,\cdot\,; d\lambda_{a,b}), \quad d\lambda_{a,b} = (t-a)(b-t)d\lambda(t). \tag{2.10}$$

It, too, is a special case of the Christoffel quadrature rule, which has an arbitrary number of prescribed nodes outside or on the boundary of the support of $d\lambda$.

2.4. The Gauss-Kronrod rule. This quadrature rule has also prescribed nodes, but they all are in the interior of the support of $d\lambda$, and it therefore transcends the class of Christoffel quadrature rules. In trying to estimate the error of the Gauss quadrature rule, Kronrod in 1964 ([12], [13]) indeed constructed a $(2n+1)$-point quadrature rule of maximum algebraic degree of exactness that has n prescribed nodes — the n Gauss nodes τ_ν^G — in addition to $n+1$ free nodes. It thus has the form

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n} \lambda_\nu^K f(\tau_\nu^G) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} f(\tau_\mu^K) + R_n^K(f). \tag{2.11}$$

Here, the node polynomial is

$$\omega_{2n+1}(t) = \pi_n(t; d\lambda)\pi_{n+1}^*(t), \quad \pi_{n+1}^*(t) = \prod_{\mu=1}^{n+1}(t - \tau_\mu^K), \tag{2.12}$$

and, according to Theorem 2.1 with n replaced by $2n+1$, the quadrature rule (2.11) has degree of exactness $d = 2n+k$ if and only if (2.11) is interpolatory and

$$\int_{\mathbb{R}} \pi_{n+1}^*(t)p(t)\pi_n(t; d\lambda)d\lambda(t) = 0 \;\text{ for all }\; p \in \mathbb{P}_{k-1}.$$

The optimal value of k is $k = n+1$, in which case π_{n+1}^* is orthogonal to all polynomials of lower degree, i.e.,

$$\pi_{n+1}^*(t) = \pi_{n+1}(t; \pi_n d\lambda). \tag{2.13}$$

That is, π_{n+1}^* is the (monic) polynomial of degree $n+1$ orthogonal relative to the oscillating measure $d\lambda_n^*(t) = \pi_n(t; d\lambda)d\lambda(t)$. While π_{n+1}^* always exists uniquely, there is no assurance that all its zeros are inside the support of $d\lambda$, or even real (cf. [5]).

3. Computation of Gauss-type quadrature rules. All quadrature rules introduced in §2 can be computed via eigenvalues and eigenvectors of a symmetric tridiagonal matrix. Part or all of this matrix is made up of the coefficients in the three-term recurrence relation satisfied by the (monic) orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; d\lambda)$ relative to the (positive) measure $d\lambda$,

$$\begin{aligned} &\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t),\ k = 0, 1, 2, \ldots, n-1, \\ &\pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \end{aligned} \tag{3.1}$$

where $\alpha_k = \alpha_k(d\lambda) \in \mathbb{R}$, $\beta_k = \beta_k(d\lambda) > 0$ depend on $d\lambda$ and $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$ by convention. The tridiagonal matrices involved are, respectively, the Jacobi, the Jacobi-Radau, the Jacobi-Lobatto, and the Jacobi-Kronrod matrix.

3.1. The Gauss quadrature rule. The Jacobi matrix of order n is defined by

$$J_n^G = J_n^G(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix}. \tag{3.2}$$

The Gauss formula (2.6) can be obtained in terms of the eigenvalues and eigenvectors of J_n^G according to the following theorem.

THEOREM 3.1. (Golub and Welsch [10]) *The Gauss nodes τ_ν^G are the eigenvalues of J_n^G, and the Gauss weights λ_ν^G are given by*

$$\lambda_\nu^G = \beta_0 [u_{\nu,1}^G]^2, \quad \nu = 1, 2, \ldots, n, \tag{3.3}$$

where u_ν^G is the normalized eigenvector of J_n^G corresponding to the eigenvalue τ_ν^G (i.e., $[u_\nu^G]^T u_\nu^G = 1$) *and $u_{\nu,1}^G$ its first component.*

Thus, to compute the nodes and weights of the Gauss formula, it suffices to compute the eigenvalues and first components of the eigenvectors of the Jacobi matrix J_n^G. Efficient methods for this, such as the QR algorithm, are well known (see, e.g., Parlett [18]). Since the first components $u_{\nu,1}^G$ of u_ν^G are easily seen to be nonzero, the positivity of the Gauss rule can be read off from (3.3).

3.2. The Gauss-Radau formula. We replace n by $n+1$ in (2.8) so as to have n interior nodes,

$$\begin{gathered} \int_{\mathbb{R}} f(t)d\lambda(t) = \lambda_0^R f(a) + \sum_{\nu=1}^{n} \lambda_\nu^R f(\tau_\nu^R) + R_{n+1}^R(f), \\ R_{n+1}^R(\mathbb{P}_{2n}) = 0. \end{gathered} \tag{3.4}$$

The Jacobi-Radau matrix of order $n+1$ is then defined by

$$J_{n+1}^R = J_{n+1}^R(d\lambda) = \left[\begin{array}{c|c} J_n^G(d\lambda) & \sqrt{\beta_n} e_n \\ \hline \sqrt{\beta_n} e_n^T & \alpha_n^R \end{array}\right], \tag{3.5}$$

where $J_n^G(d\lambda)$ is as in (3.2), $e_n^T = [0, 0, \ldots, 1]$ is the nth coordinate vector in $\mathbb{R}^n$, and

$$\alpha_n^R = a - \beta_n \frac{\pi_{n-1}(a)}{\pi_n(a)}, \tag{3.6}$$

with $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,; d\lambda)$ as before. One then has the following theorem analogous to Theorem 3.1.

THEOREM 3.2. (Golub [9]) *The Gauss-Radau nodes* $\tau_0^R = a, \tau_1^R, \ldots, \tau_n^R$ *in* (3.4) *are the eigenvalues of* J_{n+1}^R*, and the Gauss-Radau weights* λ_ν^R *are given by*

$$\lambda_\nu^R = \beta_0[u_{\nu,1}^R]^2, \quad \nu = 0, 1, 2, \ldots, n, \tag{3.7}$$

where u_ν^R *is the normalized eigenvector of* J_{n+1}^R *corresponding to the eigenvalue* τ_ν^R (i.e., $[u_\nu^R]^T u_\nu^R = 1$) *and* $u_{\nu,1}^R$ *its first component.*

As previously for the Gauss formula, the QR algorithm, now applied to J_{n+1}^R, is again the method of choice to compute Gauss-Radau formulae. Their positivity follows from (3.7). Theorem 3.2 remains in force if $a \le \inf \operatorname{supp} d\lambda$. If the right end point is the prescribed node, $\tau_{n+1}^R = b$, or if $\tau_{n+1}^R = b \ge \sup \operatorname{supp} d\lambda$, a theorem analogous to Theorem 3.2 holds with obvious changes.

3.3. The Gauss-Lobatto formula. We now replace n by $n+2$ in (2.9) and write the Gauss-Lobatto formula in the form

$$\begin{gathered}\int_{\mathbb{R}} f(t)d\lambda(t) = \lambda_0^L f(a) + \sum_{\nu=1}^{n} \lambda_\nu^L f(\tau_\nu^L) + \lambda_{n+1}^L f(b) + R_{n+2}^L(f), \\ R_{n+2}^L(\mathbb{P}_{2n+1}) = 0.\end{gathered} \tag{3.8}$$

The Jacobi-Lobatto matrix of order $n+2$ is defined by

$$J_{n+2}^L = J_{n+2}^L(d\lambda) = \left[\begin{array}{c|cc} J_n^G(d\lambda) & \sqrt{\beta_n}e_n & 0 \\ \hline \sqrt{\beta_n}e_n^T & \alpha_n & \sqrt{\beta_{n+1}^L} \\ 0^T & \sqrt{\beta_{n+1}^L} & \alpha_{n+1}^L \end{array}\right], \tag{3.9}$$

with $J_n^G(d\lambda)$ and e_n as before, and $\alpha_{n+1}^L, \beta_{n+1}^L$ the solution of the 2×2 linear system

$$\begin{bmatrix} \pi_{n+1}(a) & \pi_n(a) \\ \pi_{n+1}(b) & \pi_n(b) \end{bmatrix} \begin{bmatrix} \alpha_{n+1}^L \\ \beta_{n+1}^L \end{bmatrix} = \begin{bmatrix} a\pi_{n+1}(a) \\ b\pi_{n+1}(b) \end{bmatrix}. \tag{3.10}$$

We now have

THEOREM 3.3. (Golub [9]) *The Gauss-Lobatto nodes* $\tau_0^L = a, \tau_1^L, \ldots, \tau_n^L, \tau_{n+1}^L = b$ *in* (3.8) *are the eigenvalues of* J_{n+2}^L*, and the Gauss-Lobatto weights* λ_ν^L *are given by*

$$\lambda_\nu^L = \beta_0[u_{\nu,1}^L]^2, \quad \nu = 0, 1, 2, \ldots, n, n+1, \tag{3.11}$$

where u_ν^L *is the normalized eigenvector of* J_{n+2}^L *corresponding to the eigenvalue* τ_ν^L (i.e., $[u_\nu^L]^T u_\nu^L = 1$) *and* $u_{\nu,1}^L$ *its first component.*

Also Gauss-Lobatto formulae are therefore computable by the QR algorithm, now applied to J_{n+2}^L, and by (3.11) we still have positivity of the quadrature rule. Theorem 3.3 holds without change for $a \le \inf \operatorname{supp} d\lambda$ and $b \ge \sup \operatorname{supp} d\lambda$.

3.4. The Gauss-Kronrod formula. It has only recently been discovered by Laurie that an eigenvalue/eigenvector characterization similar to those in Theorems 3.1–3.3 holds also for the Gauss-Kronrod rule (2.11). The Jacobi-Kronrod matrix of order $2n+1$ now has the form

$$J_{2n+1}^K = J_{2n+1}^K(d\lambda) = \left[\begin{array}{c|c|c} J_n^G & \sqrt{\beta_n}e_n & 0 \\ \hline \sqrt{\beta_n}e_n^T & \alpha_n & \sqrt{\beta_{n+1}}e_1^T \\ \hline 0 & \sqrt{\beta_{n+1}}e_1 & J_n^* \end{array}\right], \tag{3.12}$$

where $e_1^T = [1, 0, \dots, 0] \in \mathbb{R}^n$ and J_n^* is a real symmetric tridiagonal matrix which has different forms depending on whether n is odd or even:

$$J^*_{n\,\mathrm{odd}} = \left[\begin{array}{c|c} J^G_{n+1:(3n-1)/2} & \sqrt{\beta_{(3n+1)/2}}e_{(n-1)/2} \\ \hline \sqrt{\beta_{(3n+1)/2}}e^T_{(n-1)/2} & J^*_{(3n+1)/2:2n} \end{array}\right], \tag{3.13}$$

$$J^*_{n\,\mathrm{even}} = \left[\begin{array}{c|c} J^G_{n+1:3n/2} & \sqrt{\beta^*_{(3n+2)/2}}e_{n/2} \\ \hline \sqrt{\beta^*_{(3n+2)/2}}e^T_{n/2} & J^*_{(3n+2)/2:2n} \end{array}\right]. \tag{3.14}$$

Here, $J^G_{p:q}$ is the principal minor matrix of the (infinite) Jacobi matrix J^G having diagonal elements $\alpha_p, \alpha_{p+1}, \dots, \alpha_q$, and $J^*_{\lfloor(3n+2)/2\rfloor:2n}$ are symmetric tridiagonal matrices, and $\beta^*_{(3n+2)/2}$ an element yet to be determined.

THEOREM 3.4. (Laurie [14]) *Let* $\lambda_\nu^K > 0$ *and* $\lambda_\mu^{*K} > 0$ *in* (2.11). *Then* J_n^* *in* (3.12) *has the same eigenvalues as* J_n^G. *Moreover, the nodes* τ_ν^G *and* τ_μ^K *are the eigenvalues of* J^K_{2n+1}, *and the Gauss-Kronrod weights are given by*

$$\lambda_\nu^K = \beta_0[u^K_{\nu,1}]^2,\ \nu = 1, \dots, n;\ \ \lambda_\mu^{*K} = \beta_0[u^K_{\mu+n,1}]^2,\ \mu = 1, \dots, n, n+1, \tag{3.15}$$

where $u_1^K, u_2^K, \dots, u^K_{2n+1}$ *are the normalized eigenvectors of* J^K_{2n+1} *corresponding to the eigenvalues* $\tau_1^G, \dots, \tau_n^G, \tau_1^K, \dots, \tau^K_{n+1}$, *and* $u^K_{1,1}, u^K_{2,1}, \dots, u^K_{2n+1,1}$ *their first components.*

Conversely, if the eigenvalues of J_n^G *and* J_n^* *are the same, then* (2.11) *exists with real nodes and positive weights.*

We remark that according to a result of Monegato [16] the positivity of λ_μ^{*K} implies the reality of the Kronrod nodes τ_μ^K and their interlacing with the Gauss nodes τ_ν^G.

Once the trailing tridiagonal blocks in (3.13), (3.14), and $\beta^*_{(3n+2)/2}$ if n is even, are known, the Gauss-Kronrod formula can be computed in much the same way as the Gauss formula in terms of eigenvalues and eigenvectors of the symmetric tridiagonal matrix J^K_{2n+1}. This in fact is the way Laurie's algorithm proceeds. Note, however, that when the nodes τ_ν^G are already known, there is a certain redundancy in this algorithm in as much as these Gauss nodes are recomputed along with the Kronrod nodes τ_μ^K. This redundancy is eliminated in a more recent algorithm of Calvetti, Golub, Gragg, and Reichel, which bypasses the computation of the trailing block in (3.12) and focuses directly onto the Kronrod nodes and weights of the Gauss-Kronrod formula.

3.4.1. Laurie's algorithm. ([14]) Assume that the hypotheses of Theorem 3.4 are fulfilled. Let, as before, $\{\pi_k\}_{k=0}^n$ denote the (monic) polynomials belonging to the Jacobi matrix $J_n^G(d\lambda)$, and thus orthogonal with respect to the measure $d\lambda$, and let $\{\pi_k^*\}_{k=0}^n$ be the (monic) orthogonal polynomials belonging to the matrix J_n^* in (3.12) and measure $d\mu^*$ (in general unknown). Define "mixed" moments by

$$\sigma_{k,\ell} = (\pi_k^*, \pi_\ell)_{d\mu^*}, \tag{3.16}$$

where $(\,\cdot\,,\,\cdot\,)_{d\mu^*}$ is the inner product relative to the measure $d\mu^*$. Although the measure $d\mu^*$ is unknown, a few things about the moments $\sigma_{k,\ell}$ are known. For example,

$$\sigma_{k,\ell} = 0 \quad \text{for } \ell < k, \tag{3.17}$$

which is an immediate consequence of orthogonality. Also,

$$\sigma_{k,n} = 0 \quad \text{for } k < n, \tag{3.18}$$

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again by orthogonality, since $\pi_n = \pi_n^*$ by Theorem 3.4. It is easy, moreover, to derive the recurrence relation

$$\sigma_{k,\ell+1} - \sigma_{k+1,\ell} - (\alpha_k^* - \alpha_\ell)\sigma_{k,\ell} - \beta_k^*\sigma_{k-1,\ell} - \beta_\ell\sigma_{k,\ell-1} = 0, \tag{3.19}$$

where $\{\alpha_k^*\}_{k=0}^{n-1}$ are the diagonal elements of J_n^* and $\{\sqrt{\beta_k^*}\}_{k=1}^{n-1}$ the elements on the side diagonals, while $\{\alpha_\ell\}_{\ell=0}^{n-1}$, $\{\sqrt{\beta_\ell}\}_{\ell=1}^{n-1}$ are the analogous elements of J_n^G. Some of the elements α_k^*, β_k^* are known according to the structure of the matrices in (3.13) and (3.14). Indeed, if we assume for definiteness that n is odd, then

$$\alpha_k^* = \alpha_{n+1+k} \text{ for } k \le (n-3)/2, \quad \beta_k^* = \beta_{n+1+k} \text{ for } k \le (n-1)/2. \tag{3.20}$$

Using the facts that $\sigma_{0,0} = \int_{\mathbb{R}} d\mu^*(t) = \beta_0^* = \beta_{n+1}$ and $\sigma_{-1,\ell} = 0$ for $\ell = 0, 1, \ldots, n-1$, $\sigma_{0,-1} = 0$, and $\sigma_{k,k-2} = \sigma_{k,k-1} = 0$ for $k = 1, 2, \ldots, (n-1)/2$, one can solve (3.19) for $\sigma_{k,\ell+1}$ and compute the entries $\sigma_{k,\ell}$ in the triangular array indicated by black dots in Fig. 3.1 (drawn for $n = 7$), since the α_k^* and β_k^* required are known by (3.20) except for the top element in the triangle. For this element the α_k^* for $k = (n-1)/2$ is not yet known, but, by good fortune, it multiplies the element $\sigma_{(n-1)/2,(n-3)/2}$, which is zero by (3.17). This mode of recursion from left to right has already been used by Salzer [21] in another context.

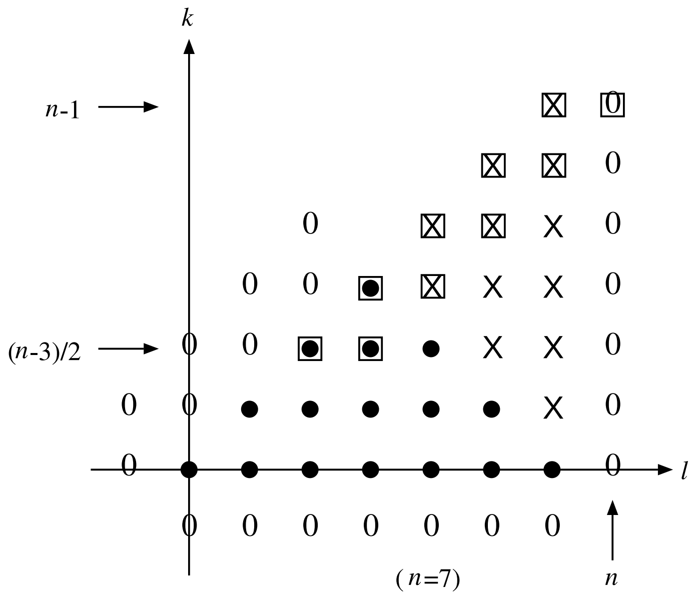

FIG. 3.1. *Computation of the mixed moments*

At this point, one can switch to a recursion from bottom up, using the recurrence relation (3.19) solved for $\sigma_{k+1,\ell}$. This computes all entries indicated by a cross in Fig. 3.1, proceeding from the very bottom to the very top of the array. For each k with $(n-1)/2 \le k \le n-1$, the entries in Fig. 3.1 surrounded by boxes are those used to compute the as yet unknown α_k^*, β_k^* according to

$$\alpha_k^* = \alpha_k + \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \quad \beta_k^* = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \tag{3.21}$$

This is the way Sack and Donovan [20] proceeded to generate modified moments in the modified Chebyshev algorithm (cf. [6, §5.2]). In the present case, crucial use is made of the property (3.18) of mixed moments, which provides the zero boundary values at the right edge of the σ-tableau. Once in possession of all the α_k^*, β_k^* required to compute J_n^*, one proceeds as described earlier.

3.4.2. The algorithm of Calvetti, Golub, Gragg, and Reichel. ([2]) Here we assume for simplicity that n is even. There is a similar, though slightly more complicated, algorithm when n is odd.

The symmetric tridiagonal matrix J_n^* in (3.12) determines its own set of orthogonal polynomials, in particular, an n-point Gauss quadrature rule relative to some (unknown) measure $d\mu^*$. Since by Theorem 3.4 the eigenvalues of J_n^* are the same as those of J_n^G, the Gauss rule in question has nodes τ_ν^G and certain positive weights μ_ν^*, $\nu = 1, 2, \ldots, n$. Likewise, the (known) matrix $J_{n+1:3n/2}^G$ of order $n/2$ in (3.14) determines another Gauss rule whose nodes and weights we denote respectively by $\tilde{\tau}_\kappa$ and $\tilde{\lambda}_\kappa$, $\kappa = 1, 2, \ldots, n/2$. Let $v = [v_1, v_2, \ldots, v_n]$ and $v^* = [v_1^*, v_2^*, \ldots, v_n^*]$ be the matrices of normalized eigenvectors of J_n^G and J_n^*, respectively. The algorithm requires the *last* components $v_{1,n}, v_{2,n}, \ldots, v_{n,n}$ of the eigenvectors $v_1, v_2, \ldots, v_n$ and the *first* components $v_{1,1}^*, v_{2,1}^*, \ldots, v_{n,1}^*$ of the eigenvectors $v_1^*, v_2^*, \ldots, v_n^*$. The latter, according to Theorem 3.1, are related to the Gauss weights μ_ν^* by means of the relation

$$\beta_0[v_{\nu,1}^*]^2 = \mu_\nu^*, \quad \nu = 1, 2, \ldots, n, \tag{3.22}$$

and can therefore be computed as the positive square roots of μ_ν^*/β_0. It can be easily shown, on the other hand, that the weights μ_ν^* are computable with the help of the second Gauss rule above as

$$\mu_\nu^* = \sum_{\kappa=1}^{n/2} \ell_\nu(\tilde{\tau}_\kappa)\tilde{\lambda}_\kappa, \quad \nu = 1, 2, \ldots, n, \tag{3.23}$$

where ℓ_ν are the elementary Lagrange polynomials associated with the nodes $\tau_1^G, \tau_2^G, \ldots, \tau_n^G$.

With these auxiliary quantities computed, the remainder of the algorithm consists of the consolidation phase of a divide-and-conquer algorithm due to Borges and Gragg ([1]). The spectral decomposition of J_n^* is

$$J_n^* = v^* D_\tau [v^*]^T, \quad D_\tau = \mathrm{diag}\,(\tau_1^G, \tau_2^G, \ldots, \tau_n^G). \tag{3.24}$$

Define

$$V := \begin{bmatrix} v & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & v^* \end{bmatrix}, \tag{3.25}$$

a matrix of order $2n+1$. We then have from (3.12) that

$$V^T(J_{2n+1}^K - \lambda I)V = \begin{bmatrix} D_\tau - \lambda I & \sqrt{\beta_n} v^T e_n & 0 \\ \sqrt{\beta_n} e_n^T v & \alpha_n - \lambda & \sqrt{\beta_{n+1}} e_1^T v^* \\ 0 & \sqrt{\beta_{n+1}} [v^*]^T e_1 & D_\tau - \lambda I \end{bmatrix}, \tag{3.26}$$

where the matrix on the right is a diagonal matrix plus a Swiss cross containing the elements of $e_n^T v$ and $e_1^T v^*$ previously computed. By orthogonal similarity transformations involving a permutation and a sequence of Givens rotations, the matrix in (3.26) can be reduced to the form

$$\tilde{V}^T(J^K_{2n+1} - \lambda I)\tilde{V} = \left[\begin{array}{c|cc} D_\tau - \lambda I & 0 & 0 \\ \hline 0 & D_\tau - \lambda I & c \\ 0 & c^T & \alpha_n - \lambda \end{array}\right], \tag{3.27}$$

where $\tilde{V}$ is the transformed matrix V and c a vector containing the entries in positions $n+1$ to $2n$ of the transformed vector $[\sqrt{\beta_n}e_n^T v, \sqrt{\beta_{n+1}}e_1^T v^*, \alpha_n]$. It is now evident from (3.27) that one set of eigenvalues of J^K_{2n+1} is $\{\tau_1^G, \tau_2^G, \ldots, \tau_n^G\}$. The remaining eigenvalues are those of the trailing block in (3.27). To compute them, observe that

$$\begin{bmatrix} D_\tau - \lambda I & c \\ c^T & \alpha_n - \lambda \end{bmatrix} = \begin{bmatrix} I & 0 \\ c^T(D_\tau - \lambda I)^{-1} & 1 \end{bmatrix} \begin{bmatrix} D_\tau - \lambda I & c \\ 0^T & -f(\lambda) \end{bmatrix},$$

where in terms of the components c_ν of c,

$$f(\lambda) = \lambda - \alpha_n + \sum_{\nu=1}^{n} \frac{c_\nu^2}{\tau_\nu^G - \lambda}. \tag{3.28}$$

Thus, the remaining eigenvalues of J^K_{2n+1} are the zeros of $f(\lambda)$, which can be seen to interlace with the nodes τ_ν^G. The first components of the normalized eigenvectors $u_1^K, u_2^K, \ldots, u_{2n+1}^K$ needed according to Theorem 3.4 are also computable from the columns of V by keeping track of the orthogonal transformations.

4. Quadrature rules with multiple nodes. We now consider quadrature rules of the form

$$\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n}\sum_{\rho=0}^{r-1} \lambda_\nu^{(\rho)} f^{(\rho)}(\tau_\nu) + R_n(f), \tag{4.1}$$

where each τ_ν is a node of multiplicity r. The underlying interpolation process is the one of Hermite, which is exact for polynomials of degree $\leq r \cdot n - 1$. We therefore call (4.1) interpolatory if it has degree of exactness $d = r \cdot n - 1$. As before, the node polynomial is defined by

$$\omega_n(t) = \prod_{\nu=1}^{n} (t - \tau_\nu). \tag{4.2}$$

In analogy to Theorem 2.1, we now have the following theorem.

THEOREM 4.1. *The quadrature rule* (4.1) *has degree of exactness* $d = r \cdot n - 1 + k$, $k \geq 0$, *if and only if both of the following conditions are satisfied:*

(a) *the formula* (4.1) *is interpolatory;*

(b) *the node polynomial* ω_n *satisfies*

$$\int_{\mathbb{R}} [\omega_n(t)]^r p(t) d\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{k-1}. \tag{4.3}$$

The case $k = 0$ corresponds to the Newton-Cotes-Hermite formula, which requires no extra condition beyond that of being interpolatory. If $k > 0$, the condition (b) is again a condition involving only the nodes τ_ν, namely orthogonality of the rth power of ω_n to all polynomials of degree $\leq k-1$. It is immediately clear from (4.3) that for positive measures $d\lambda$ the multiplicity r must be an odd integer, since otherwise we could not have orthogonality of ω_n^r to a constant, let alone to $\mathbb{P}_{k-1}$. It is customary, therefore, to write

$$r = 2s+1, \quad s \geq 0. \tag{4.4}$$

It then follows that $k \leq n$, since otherwise $k = n+1$ would imply orthogonality of ω_n^r to all polynomials of degree $\leq n$, in particular, orthogonality to ω_n, which, r being odd, is impossible. Thus, $k = n$ is optimal; the corresponding interpolatory quadrature rule is called the Gauss-Turán rule for the measure $d\lambda$ ([22]). For it, the polynomial ω_n^{2s+1} is orthogonal to all polynomials of degree $\leq n-1$, the polynomial ω_n thus the so-called s-orthogonal polynomial of degree n. There is an extensive theory of these polynomials, for which we refer to the book of Ghizzetti and Ossicini [8, §§3.9,4.13]. We mention here only the elegant result of Turán [22], according to which ω_n is the extremal polynomial of

$$\int_{\mathbb{R}} [\omega(t)]^{2s+2} d\lambda(t) = \min, \tag{4.5}$$

where the minimum is sought among all monic polynomials ω of degree n. From this, there follows in particular the existence and uniqueness of real Gauss-Turán formulae, but not necessarily their positivity. Nevertheless, it has been shown by Ossicini and Rosati [17] that $\lambda_\nu^{(\rho)} > 0$, $\nu = 1, 2, \ldots, n$, if $\rho \geq 0$ is even.

5. Computation of Gauss-Turán quadrature rules. (Gautschi and Milovanović [7]) The computation of the Gauss-Turán formula

$$\begin{gathered}\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{\nu=1}^{n}\sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)T} f^{(\sigma)}(\tau_\nu^T) + R_n^T(f), \\ R_n^T(\mathbb{P}_{2(s+1)n-1}) = 0,\end{gathered} \tag{5.1}$$

involves two stages:

(i) The generation of the s-orthogonal polynomial $\pi_n = \pi_{n,s}$, i.e., the polynomial π_n satisfying the orthogonality relation

$$\int_{\mathbb{R}} [\pi_n(t)]^{2s+1} p(t) d\lambda(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}; \tag{5.2}$$

the zeros of π_n are the desired nodes τ_ν^T in (5.1).

(ii) The computation of the weights $\lambda_\nu^{(\sigma)T}$.

Since the latter stage requires knowledge of the nodes τ_ν^T, we begin with the computation of the s-orthogonal polynomial $\pi_{n,s}$.

We reinterpret power orthogonality in (5.2) as ordinary orthogonality with respect to the measure

$$d\lambda_{n,s}(t) = [\pi_n(t)]^{2s} d\lambda(t), \tag{5.3}$$

which, like $d\lambda$, is also positive,

$$\int_{\mathbb{R}} \pi_n(t) p(t) d\lambda_{n,s}(t) = 0 \quad \text{for all } p \in \mathbb{P}_{n-1}. \tag{5.4}$$

Since the measure $d\lambda_{n,s}$ involves the unknown π_n, one also talks about implicit orthogonality.

The measure $d\lambda_{n,s}$ being positive, it defines a sequence $\pi_k(t) = \pi_k(t; d\lambda_{n,s})$, $k = 0, 1, \dots, n$, of orthogonal polynomials, of which only the last one for $k = n$ is of interest to us. They satisfy a three-term recurrence relation (3.1), with coefficients α_k, β_k given by the well-known inner product formulae

$$\begin{aligned} &\alpha_k = \frac{\int_{\mathbb{R}} t\pi_k^2(t) d\lambda_{n,s}(t)}{\int_{\mathbb{R}} \pi_k^2(t) d\lambda_{n,s}(t)}, \quad k = 0, 1, \dots, n-1, \\ &\beta_0 = \int_{\mathbb{R}} d\lambda_{n,s}(t), \quad \beta_k = \frac{\int_{\mathbb{R}} \pi_k^2(t) d\lambda_{n,s}(t)}{\int_{\mathbb{R}} \pi_{k-1}^2(t) d\lambda_{n,s}(t)}, \\ &\qquad\qquad\qquad\qquad k = 1, \dots, n-1. \end{aligned} \tag{5.5}$$

This constitutes a system of $2n$ nonlinear equations for the $2n$ coefficients $\alpha_0, \alpha_1, \dots, \alpha_{n-1}; \beta_0, \beta_1, \dots, \beta_{n-1}$, which can be written in the form

$$\phi = 0, \quad \phi^T = [\phi_0, \phi_1, \dots, \phi_{2n-1}], \tag{5.6}$$

where, in view of (5.3),

$$\begin{aligned} &\phi_0 := \beta_0 - \int_{\mathbb{R}} \pi_n^{2s}(t) d\lambda(t), \\ &\phi_{2\nu} := \int_{\mathbb{R}} [\beta_\nu \pi_{\nu-1}^2(t) - \pi_\nu^2(t)] \pi_n^{2s}(t) d\lambda(t), \ \nu = 1, \dots, n-1, \\ &\phi_{2\nu+1} := \int_{\mathbb{R}} (\alpha_\nu - t) \pi_\nu^2(t) \pi_n^{2s}(t) d\lambda(t), \ \nu = 0, 1, \dots, n-1. \end{aligned} \tag{5.7}$$

Here, each π_k is to be considered a function of $\alpha_0, \dots, \alpha_{k-1}; \beta_1, \dots, \beta_{k-1}$ by virtue of the three-term recurrence relation (3.1) which it satisfies. Since all integrands in (5.7) are polynomials of degree $\le 2(s+1)n - 1$, the integrals in (5.7) can be computed exactly by an $(s+1)n$-point Gaussian quadrature rule relative to the measure $d\lambda$. Any method for solving systems of nonlinear equations, such as Newton's method or quasi-Newton methods, can now be applied to solve (5.6). (For Newton's method, in this context, see [7].)

We now turn to the computation of the quadrature weights. Here we note that

$$\begin{aligned} &\omega_{\rho,\nu}(t) = (t - \tau_\nu^T)^\rho \prod_{\mu \ne \nu} (t - \tau_\mu^T)^{2s+1}, \\ &\qquad\qquad \rho = 0, 1, \dots, 2s; \ \nu = 1, \dots, n, \end{aligned} \tag{5.8}$$

are polynomials of degree $\le (2s+1)n - 1$, hence, by (5.1), $R_n^T(\omega_{\rho,\nu}) = 0$. This can be written as

$$\sum_{\kappa=1}^{n} \sum_{\sigma=0}^{2s} \lambda_\kappa^{(\sigma)T} \omega_{\rho,\nu}^{(\sigma)}(\tau_\kappa^T) = b_{\rho,\nu}, \tag{5.9}$$

with

$$b_{\rho,\nu} = \int_{\mathbb{R}} \omega_{\rho,\nu}(t) d\lambda(t). \tag{5.10}$$

By virtue of the definition (5.8) of $\omega_{\rho,\nu}$, we have $\omega_{\rho,\nu}^{(\sigma)}(\tau_\kappa^T) = 0$ for $\kappa \ne \nu$, so that the system (5.9) breaks up into n separate linear systems for the weights $\lambda_\nu^{(\sigma)T}$, $\sigma = 0, 1, \dots, 2s$,

$$\sum_{\sigma=0}^{2s} \lambda_\nu^{(\sigma)T} \omega_{\rho,\nu}^{(\sigma)}(\tau_\nu^T) = b_{\rho,\nu}, \quad \rho = 0, 1, \dots, 2s. \tag{5.11}$$

Each of these systems further simplifies since $\omega_{\rho,\nu}^{(\sigma)}(\tau_\nu^T) = 0$ for $\rho > \sigma$. That is, for each ν, we obtain the upper triangular system

$$\begin{bmatrix} \omega_{0,\nu}(\tau_\nu^T) & \omega'_{0,\nu}(\tau_\nu^T) & \cdots & \omega_{0,\nu}^{(2s)}(\tau_\nu^T) \\ & \omega'_{1,\nu}(\tau_\nu^T) & \cdots & \omega_{1,\nu}^{(2s)}(\tau_\nu^T) \\ & & \ddots & \vdots \\ & & & \omega_{2s,\nu}^{(2s)}(\tau_\nu^T) \end{bmatrix} \begin{bmatrix} \lambda_\nu^{(0)T} \\ \lambda_\nu^{(1)T} \\ \vdots \\ \lambda_\nu^{(2s)T} \end{bmatrix} = \begin{bmatrix} b_{0,\nu} \\ b_{1,\nu} \\ \vdots \\ b_{2s,\nu} \end{bmatrix}. \tag{5.12}$$

The matrix elements can easily be computed by linear recursions (cf. [7]) and the elements of the right-hand vector by $(s+1)n$-point Gauss quadrature as before.

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