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A NOTE ON POSITIVE QUADRATURE RULES

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ABSTRACT. A classical problem in constructive function theory is the characterization of positive quadrature rules by linear combinations of orthogonal polynomials the roots of which determine the nodes of the formula. A complete characterization has been derived by F. Peherstorfer in 1984. In this note a variant to his approach will be discussed. It is the one-dimensional restriction of a characterization of interpolatory cubature formulae which might be of some general interest.

1. Introduction. We denote $\mathbf{P}$ the ring of real polynomials in one variable and by $\mathbf{P}[a,b]$ the restriction of $\mathbf{P}$ to $[a,b] \subseteq \mathbf{R}$. The linear space spanned by $\{1, x, x^2, \ldots, x^m\}$ will be denoted by $\mathbf{P}_m$.

Let

$$I : \mathbf{P}[a,b] \to \mathbf{R} : f \to I(f),\ I(1) = 1,$$

be a strictly positive linear functional, i.e., I is linear and $f \geq 0$ implies $I(f) > 0$ for all $f \in \mathbf{P}[a,b], f \neq 0$. Thus I represents those functionals usually studied in numerical integration.

We denote by p_i the orthogonal polynomials of degree i with respect to I, normalized such that the highest coefficient is 1, i.e.,

$$p_i = id^i + \sum_{j=0}^{i-1} \alpha_j id^j$$

such that $I(fp_i) = 0$ for all $f \in \mathbf{P}_{i-1}$. These polynomials satisfy the recursion formula

$$(1)\quad p_0 = 1,\ p_1 = id - \Gamma_0,\ p_{i+1} = (id - \Gamma_i)p_i - \Lambda_i p_{i-1}, i = 1, 2, \ldots,$$

where

$$\Gamma_0 = I(id),\ \Lambda_0 = 1,\ \Gamma_i = \frac{I(idp_i^2)}{I(p_i^2)},\ \Lambda_i = \frac{I(p_i^2)}{I(p_{i-1}^2)},\ i = 1, 2, \ldots .$$

In addition we use the notation

$$G_i = I(p_i^2) = \Lambda_0\Lambda_1 \dots \Lambda_i > 0, \;\; i = 0, 1, \dots .$$

The linear functional
(2)

$$Q : \mathbf{P} \to \mathbf{R} : f \to Q(f) = \sum_{i=1}^{k} c_i f(x_i), \quad c_i > 0, \;\; x_i \in [\alpha, \beta], \;\; x_i \neq x_j,$$

is called a positive quadrature rule of type (m, k) for I with nodes in $[\alpha, \beta]$, if $I(f) = Q(f)$ for all $f \in \mathbf{P}_m$ and $I(id^{m+1}) \neq Q(id^{m+1})$ hold. Many applications require that the nodes x_i belong to $[a, b]$.

By the strict positivity of I we obtain the classical lower bound $k \geq [m/2] + 1$ for a quadrature rule (2) of degree m. Hence we can consider formulae of type $(2k - s, k)$, $s = 1, 2, \dots, k + 1$. For $s = 1$ we obtain Gaussian formulae, for $s = 2$ formulae of Radau-type. The Lobatto-type case has been studied by L. Féjer [**1**] and was treated completely by C.A. Micchelli and T.J. Rivlin [**2**]. The general case, finally, has been characterized completely by F. Peherstorfer [**4**]. For the historical development and further approaches we refer to [**3, 7** and **8**].

We present the one-dimensional case of a characterization of interpolatory cubature formulae. The one-dimensional case is easy to derive and allows control of the distribution of the nodes.

2. Characterization. Let (2) be a quadrature rule of type $(2k - s, k)$. Then the polynomial $q = (id - x_1)(id - x_2) \dots (id - x_k)$ vanishes at the nodes of q. Since the coefficients c_i are uniquely determined by the nodes, the roots of q determine the formula, or, more briefly, q generates the quadrature rule. Due to the degree of exactness q must be orthogonal to $\mathbf{P}_{k-s}$ with respect to I, hence

$$q = p_k + \sum_{i=1}^{s-1} \gamma_{s-i} p_{k-i}, \quad \gamma_i \in \mathbf{R}, \;\; \gamma_1 \neq 0. \tag{3}$$

To obtain the prescribed degree of exactness we must require $\gamma_1 \neq 0$. We shall study under which conditions on the γ_i's the polynomial q in

(3) generates a positive quadrature rule of type $(2k - s, k)$ for I with nodes in $[\alpha, \beta]$, thus characterizing all formulae of this type.

Let q be an arbitrary polynomial of degree k, we denote by

$$\Pi_q : \mathbf{P} \to \mathbf{P}_{k-1} : f \to \Pi_q(f)$$

the linear projection from $\mathbf{P}$ to $\mathbf{P}_{k-1}$ with respect to q, defined by the unique representation of f as $f = rq + \prod_q(f)$, $r \in \mathbf{P}$, $\prod_q(f) \in \mathbf{P}_{k-1}$. For the strictly positive linear functional I on $\mathbf{P}[a,b]$ we define an associated linear functional depending on q by

$$I_q : \mathbf{P} \to \mathbf{R} : f \to I_q(f) = I(\Pi_q(f)).$$

These definitions allow the following characterization of positive quadrature rules.

THEOREM. *Let I be a strictly positive linear functional on $\mathbf{P}[a,b]$. For a given $s, 1 \leq s \leq k+1$, let q be of the form* (3). *Then q generates a positive quadrature rule of type $(2k - s, k)$ for I if and only if I_q is strictly positive on $\mathbf{P}_{2k-1}$.*

PROOF. ($\Rightarrow$). Let (2) be a positive quadrature rule of type $(2k-s, k)$ for I which is generated by q. Every nonnegative polynomial $f \in \mathbf{P}_{2k-1}$ can be written as $f = p_1^2 + p_2^2$, $p_1, p_2 \in \mathbf{P}_{k-1}$. So a nonnegative $f \in \mathbf{P}_{2k-1}$, $f \neq 0$, cannot vanish all nodes of (2), and we find

$$I_q(f) = I(\Pi_q(f)) = I(f - rq) = \sum_{i=1}^{k} c_i f(x_i) > 0,$$

where $r \in \mathbf{P}_{k-1}$ is chosen such that $f - rq \in \mathbf{P}_{k-1}$. Hence I_q is strictly positive on $\mathbf{P}_{2k-1}$.

($\Leftarrow$). If I_q is strictly positive on $\mathbf{P}_{2k-1}$, then q is the k-th orthogonal polynomial with respect to I_q, since $I_q(gq) = 0$ for all $g \in \mathbf{P}_{k-1}$. So q generates the Gaussian formula of degree $2k-1$ for I_q. Since q is orthogonal to $\mathbf{P}_{k-s}$ with respect to I, we find for all $f \in \mathbf{P}_{2k-s}$ the relation

$$I_q(f) = I(\Pi_q(f)) = I(f - rq) = I(f),$$

where $r \in \mathbf{P}_{k-s}$ is chosen such that $f - rq \in \mathbf{P}_{k-1}$. Hence the Gaussian formula for I_q is a positive quadrature rule of type $(2k - s, k)$ for I.□

The Theorem is the one-dimensional case of a characterization of interpolatory cubature formulae, see [**6**, Theorem 3.4.1]. The proof via projections is due to G. Renner [**5**]. In contrast to the multivariate case the proof can be reduced to elementary facts of Gaussian quadrature which are not available in the general case.

Let q be of the form (3) and let I_q be strictly positive on $\mathbf{P}_{2k-1}$. We denote by $q_i, i = 0, 1, \ldots, k$, the orthogonal polynomials with respect to I_q. The recursion for the q_i's is of the form

(4) $q_{i+1} = (id - \Gamma_i^*)q_i - \Lambda_i^* q_{i-1}, \; \Gamma_i^* \in \mathbf{R}, \; \Lambda_i > 0, \; i = 0, 1, \ldots, k-1,$

Since $I_q = I$ on $\mathbf{P}_{2k-s}$ we obtain

$$q_i = p_i, \; i = 0, 1, \ldots, k - [s/2], \tag{5}$$

furthermore, $q_k = q$.

Thus quadrature rules of type $(2k-s, k)$ for I are generated by $q = q_k$, the k-th orthogonal polynomial with respect to I_q. It can be computed recursively via (5) and (4) for arbitrarily chosen $\Lambda_i^* > 0$, $\Gamma_i^* \in \mathbf{R}$, $i = k - [s/2], k - [s/2] + 1, \ldots, k - 1$. This is F. Peherstorfer's elegant characterization. The distribution of the roots of q can be controlled by Sturm's Theorem applied to $\{q_i\}_{i=0,1,\ldots,k}$. This is a characterization of the strict positivity of I_q by the recursion (4). In order to get a characterization by the coefficients of q - similar to the approach by G. Sottas and G. Wanner [**7**] - we shall present a direct application of the Theorem.

3. Application. The strict positivity of I_q on $\mathbf{P}_{2k-1}$ will be expressed in terms of the γ_i's in (3), while the distribution of the roots of q will be controlled by the Sturm-sequence of the orthogonal polynomials with respect to I_q.

Let us assume that q is of the form (3) for a given $s, 1 \leq s \leq k+1$. The strict positivity of I_q on $\mathbf{P}_{2k-1}$ is characterized by $I_q(p^2) > 0$ for all $p \in \mathbf{P}_{k-1}, p \neq 0$. Assuming

$$p = \sum_{i=0}^{k-1} \lambda_i p_i, \; \lambda_i \in \mathbf{R}, \; \sum_{i=0}^{k-1} \lambda_i^2 > 0,$$

the strict positivity of I_q is equivalent to

$$I_q(p^2) = \sum_{i=0}^{k-1} \sum_{j=1}^{k-1} \lambda_i \lambda_j I_q(p_i p_j) > 0$$

for the described set of λ_i's. Hence I_q is strictly positive on $\mathbf{P}_{2k-1}$ if and only if

$$T = (I_q(p_i p_j))_{i,j=0,1,\ldots,k-1}$$

is positive definite. So we have to compute the entries t_{ij} of the $k \times k$ matrix T (depending on the γ_i's) and study the positive definiteness of T. For the computation we use the following

LEMMA. *Let $p_i, p_j, 0 \leq i, j \leq k-1$ be given. Then $t_{ij} = I_q(p_i p_j) = I(p_i p_j - r_{ij} q)$, where r_{ij} is arbitrarily chosen in $\mathbf{P}_{k-s}$ such that*

$$g_{ij} = p_i p_j - r_{ij} q \in \mathbf{P}_{2k-s}. \tag{6}$$

PROOF. Since $I_q(f) = I(f)$ for all $f \in \mathbf{P}_{2k-s}$ we get, for g_{ij} satisfying (6), the relation

$$I(g_{ij}) = I(p_i p_j - r_{ij} q) = I_q(p_i p_j - r_{ij} q) = I_q(p_i p_j) = t_{ij}.$$

Let G be a $k \times k$ matrix with entries as defined in (6). If $0 \leq i + j \leq 2k - s$ we can choose $r_{ij} = 0$, hence $g_{ij} = p_i p_j$. So the first row and column of G are known. If row $i-1$ of G has already been determined, we define, in addition,

$$g_{i-1,k} = -\sum_{j=1}^{s-1} \gamma_{s-j} g_{i-1,k-j} \in \mathbf{P}_{2k-s}.$$

This polynomial satisfies (6) since it can be written as $g_{i-1,k} = p_{i-1} p_k - q r_{i-1,k}$, where

$$r_{i-1,k} = p_{i-1} - \sum_{j=1}^{s-1} \gamma_{s-j} r_{i-1,k-j}.$$

To compute the element of the i-th row of G we insert the recursion (1) for p_i and p_{j+1} obtaining

$$p_i p_j = p_{i-1}p_{j+1} + (\Gamma_j - \Gamma_{i-1})p_{i-1}p_j + \Lambda_j p_{i-1}p_{j-1} - \Lambda_{i-1}p_{i-2}p_j.$$

This implies

$$\begin{aligned} g_{ij} &= g_{i-1,j+1} + (\Gamma_j - \Gamma_{i-1})g_{i-1,j} + \Lambda_j g_{i-1,j-1} - \Lambda_{i-1}g_{i-2,j} \\ &= p_i p_j - r_{ij}q, \ j = 0, 1, \dots, k-1, \end{aligned}$$

where $r_{ij} = r_{i-1,j+1} + (\Gamma_j - \Gamma_{i-1})r_{i-1,j} + \Lambda_j r_{i-1,j-1} - \Lambda_{i-1}r_{i-2,j}$. Since the recursions for g_{ij} are linear we directly obtain the following recursions for the entries of T:

$$\begin{aligned} &t_{ij} = G_i\delta_{ij}, \ 0 \le i+j \le 2k-s, \\ (7) \quad &t_{i-1,k} = -\sum_{j=1}^{s-1}\gamma_{s-j}t_{i-1,k-j}, \ i = k-s+1, k-s+2, \dots, k-1, \\ &t_{i-1,k} = t_{i-1,j+1} + (\Gamma_j - \Gamma_{i-1})t_{i-1,j} + \Lambda_j t_{i-1,j-1} - \Lambda_{i-1}t_{i-2,j}, \\ &\qquad i, j = k-s+2, k-s+3, \dots, k-1. \end{aligned}$$

Hence T can be written as

$$T = \begin{pmatrix} D & 0 \\ 0 & S \end{pmatrix},$$

where $D = \operatorname{diag}\{G_0, G_1, \dots, G_{k-s+1}\}$ and

$$S = \begin{pmatrix} G_{k-s+2} & 0 & 0 & \dots & 0 & 0 & -\gamma_1 G_{k-s+1} \\ 0 & G_{k-s+3} & 0 & \dots & 0 & * & * \\ 0 & 0 & G_{k-s+4} & \dots & * & * & * \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & * & \dots & * & * & * \\ 0 & * & * & \dots & * & * & * \\ -\lambda_1 G_{k-s+1} & * & * & \dots & * & * & * \end{pmatrix}$$

T is positive definite if and only if the $(s-2) \times (s-2)$ submatrix S is positive definite. Let us denote the elements of S by σ_{ij}. The first row and column of S are known. The remaining entries are computed from the recursion (7) as

$$(8)\quad \begin{aligned}&\sigma_{ij} = \sigma_{i-1,j+1} + (\Gamma_j - \Gamma_{i-1})\sigma_{i-1,j} + \Lambda_j\sigma_{i-1,j-1} - \Lambda_{i-1}\sigma_{i-2,j},\\ &\sigma_{k-s+1,j} = 0,\ i,j = k-s+3, k-s+4, \ldots, k-1.\end{aligned}$$

The elements of $\sigma_{i,k}, i = k-s+3, k-s+4, \ldots, k-2$, are computed successively from

$$(9)\qquad \begin{pmatrix} \sigma_{k-s+2,k} \\ \sigma_{k-s+3,k} \\ \vdots \\ \sigma_{k-1,k} \end{pmatrix} = -S \begin{pmatrix} \gamma_2 \\ \gamma_3 \\ \vdots \\ \gamma_{s-1} \end{pmatrix}.$$

The symmetry of S is useful for the calculation. For $s = 2$ we obtain

$$T = \operatorname{diag}\{G_0, G_1, \ldots, G_{k-1}\}$$

which is obviously positive definite. For $s = 3$ we obtain

$$S + (G_{k-1} - \gamma_1 G_{k-2}),$$

finally, for $s = 4$ we get

$$S = \begin{pmatrix} G_{k-2} & -\gamma_1 G_{k-3} \\ -\gamma_1 G_{k-3} G_{k-1} - G_{k-2\gamma_2} + G_{k-3\gamma_1\gamma_3} - & (\Gamma_{k-1} - \Gamma_{k-2}) G_{k-3\gamma_1} \end{pmatrix}.$$

The computation becomes loathsome with increasing s. The positive definiteness of S restricts the $\gamma_i s$ such that the corresponding q generates a positive quadrature rule for I with real nodes. This is the one-dimensional case of the characterization given in [**6**] being equivalent to the conditions derived in [**7**].

To control the distribution of the nodes we use the polynomials q_i which are orthogonal with respect to I_q. Let us assume

$$q_i = p_i + \sum_{j=0}^{i-1} \delta_j p_j,\ \delta_j \in \mathbf{R},\ i = 0, 1, \ldots, k-1.$$

Then $I_q(q_i p_j) = 0$ for $j = 0, 1, \ldots, i-1$ is equivalent to

$$S \begin{pmatrix} \delta_{k-s+2} \\ \vdots \\ \delta_{i-1} \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = 0, \; i = k - [s/2] + 1, \; k - [s/2] + 2, \ldots, k-1.$$

Since I_q is strictly positive on $\mathbf{P}_{2k-1}$, q has k pairwise distinct real roots and the q_i's form a Sturm-sequence. By Sturm's Theorem q has its real roots in $[\alpha, \beta]$ if and only if

$$\begin{gathered} q(\beta) \geq 0, \; (-1)^k q(\alpha) \geq 0, \; q_i(\beta) > 0, \; (-1)^i q_i(\beta) > 0, \\ i = 0, 1, \ldots, k-1. \end{gathered} \tag{10}$$

4. Examples. Let us characterize the first simple cases of positive quadrature rules of type $(2k - s, k)$ with nodes in $[a, b]$. For $s = 2, 3, 4$ we have computed above the $(s-2) \times (s-2)$ matrices S using (8) and (9). The positive definiteness of these matrices and (10) lead to the following results.

Rules of type $(2k-2, k)$ are generated by $q = p_k + \gamma_1 p_{k-1}$, where $q(b) \geq 0$, $(-1)^k q(a) \geq 0$. Rules of type $(2k-3, k)$ are generated by $q = p_k + \gamma_2 p_{k-1} + \gamma_1 p_{k-2}$, where

$$\gamma_1 < \Lambda_{k-1}, \qquad q(b) \geq 0, \qquad (-1)^k q(a) \geq 0.$$

Rules of type $(2k-4, k)$ are generated by $q = p_k + \gamma_3 p_{k-1} + \gamma_2 p_{k-2} + \gamma_1 p_{k-3}$, where

$$\Lambda_{k-2}^2(\Lambda_{k-1} - \gamma_2) + \Lambda_{k-2}\gamma_1\gamma_3 + (\Gamma_{k-1} - \Gamma_{k-2})\Lambda_{k-2}\gamma_1 - \gamma_1^2 > 0$$

and

$$q(b) \geq 0, \quad (-1)^k q(a) \geq 0, \quad q_{k-1}(b) > 0, \quad (-1)^{k-1} q_{k-1}(a) > 0,$$

with

$$q_{k-1} = p_{k-1} + \frac{\gamma_1}{\Lambda_{k-2}} p_{k-2}.$$

These are the cases which are easy to derive. The amount of computational work increases rapidly with s. Further computation in this general set-up should be done using a computer-algebra system.

If a special form of the generating polynomial q is of interest our approach seems to be easier to apply. We shall illustrate this by the following example.

The polynomial

$$q = p_k + \gamma_1 p_{k-s+1}, \ \gamma_1 \neq 0, \tag{11}$$

generates a positive quadrature rule of type $(2k - s, k)$ if $|\gamma_1|$ is sufficiently small. Exact bounds can be determined easily in special cases, e.g., if I is chosen such that

$$\Lambda_i = \Lambda, \ \Gamma_i = \Gamma, \ i = k-s+2, k-s+3, \ldots, k-1.$$

The Chebyshev-polynomials of the first and second kind (Λ_1 is $1/2$ or $1/4$, respectively) satisfy (1) with $\Gamma_i = 0$, $\Lambda_2 = \Lambda_3 = \cdots = 1/4$. So they belong to a functional of the appropriate class of $s \leq k$. For such a functional I and a polynomial q of type (11) the recursion (8) is reduced to

$$\begin{aligned}
&\sigma_{ij} = \sigma_{i-1,j+1} + \Lambda(\sigma_{i-1,j-1} - \sigma_{i-2,j}),\\
&\sigma_{ik} = 0, \ \sigma_{k-s+1,j} = 0, \ i,j = k-s+3, k-s+4, \ldots, k-1.
\end{aligned}$$

For $4 \leq s \leq k$ the matrix S is up to a positive factor of the form

$$S = \begin{pmatrix} \Lambda & 0 & \ldots & 0 & -\gamma_1 \\ 0 & \Lambda^2 & \ldots & -\gamma_1 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ -\gamma_1 & 0 & \ldots & 0 & \Lambda^{s-2} \end{pmatrix},$$

hence it is positive definite if and only if $\gamma_1^2 < \Lambda^{s-1}$. The orthogonal polynomials with respect to I_q are of the form

$$q_{k-1} = p_{k-i} + \frac{\gamma_1}{\Lambda^i} p_{k-s+i+1}, \ i = 0, 1, \ldots, [s/2] - 1,$$

so the condition (10) can be checked quite easily. If we select the Chebyshev-polynomials of the first and second kind, respectively, the roots of q are in $(-1, 1)$ if $\gamma_1^2 < \Lambda^{s-1}$.

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