Finite Sequences of Orthogonal Polynomials Connected by a Jacobi Matrix

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ABSTRACT

If $p_0, \dots, p_n$ is an orthogonal sequence, with p_j a monic polynomial of exact degree j, all j, then the sequence $q_0, \dots, q_n$ of monic polynomials defined by the requirement that $p_j = c_j q_{n-j-1} p_{n-1}$ at the zeros of p_n (with c_j suitable constants) is also orthogonal (with respect to a possibly differently weighted scalar product). These two sequences can be shown to be the upper left, respectively lower right, principal minors of the matrix $t - J$, with J a suitable tridiagonal matrix. The sequence q occurs in the characterization of the discrete least-squares approximation to f from $\operatorname{span}(p_0, \dots, p_j)$ in terms of the $(n-j-1)$-order divided differences of f/p_{n-1} at the nodes, i.e., the zeros of p_n. A complete characterization of the pair (U, V) of zero sets of p_{j-1} and q_{n-j} is given, and an application is made to the problem of recovering a Jacobi matrix from such data.

0. INTRODUCTION

The connection between two finite sequences of orthogonal polynomials mentioned in the title arose in the following way. Consider least squares rational approximation to a function $f(z)$ analytic on the closed unit disk in the z-plane. Given n points $\beta_1, \beta_2, \dots, \beta_n$ exterior to the unit circle, we wish

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to determine the rational function

$$\hat{r}_m(z) = \frac{\hat{p}_m(z)}{\prod_1^n (z - \beta_i)}$$

that minimizes the integral

$$\int_{|z|=1} |f(z) - r_m(z)|^2 |dz|$$

over all rational functions r_m of the form

$$r_m(z) = \frac{p_m(z)}{\prod_1^n (z - \beta_i)}, \qquad p_m \in \pi_m,$$

where π_m denotes the collection of all polynomials of degree at most m. An elegant theorem of J. L. Walsh [W, p. 244] asserts that, for $m \geqslant n$, the least squares approximant $\hat{r}_m$ must interpolate f in the $m+1$ zeros of the polynomial $z^{m-n+1}\Pi_1^n(z - 1/\bar{\beta}_i)$. Although Walsh does not discuss the determination of $\hat{r}_m$ in the case when $m < n$, his proof leads immediately to the following characterization, which is stated in terms of divided differences. Namely, if $0 \leqslant m < n$, then $\hat{r}_m$ satisfies

$$\left[\frac{1}{\bar{\beta}_{j+1}}, \dots, \frac{1}{\bar{\beta}_{j+n-m}}\right] z^{n-m-1} f(z) = \left[\frac{1}{\bar{\beta}_{j+1}}, \dots, \frac{1}{\bar{\beta}_{j+n-m}}\right] z^{n-m-1} \hat{r}_m(z),$$
$$j = 0, \dots, m. \qquad (0.1)$$

A natural question which arises is this: Is there an analogue of the conditions (0.1) in the case of weighted least squares *polynomial approximation in n distinct real points*?

An answer to this question is provided below in Proposition 1 in terms of the associated sequence $(p_i)_0^n$ of monic orthogonal polynomials and a second sequence $(q_i)_0^n$ of monic polynomials. The latter are given by the condition that on the n points,

$$c_j q_{n-j-1} = p_j / p_{n-1}$$

for some constant c_j.

As it turns out, the connection between these two polynomial sequences has been noted and used before, in [BG], in the study of the numerical reconstruction of a Jacobi matrix from certain spectral data. To recall, by a *Jacobi* matrix is meant a tridiagonal matrix of the form

$$J = \begin{bmatrix} a_1 & b_1 & & & & & \\ b_1 & a_2 & b_2 & & & & \\ & b_2 & a_3 & b_3 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & b_{n-2} & a_{n-1} & b_{n-1} \\ & & & & & b_{n-1} & a_n \end{bmatrix}, \tag{0.2}$$

where J is real and the next-to-diagonal elements are positive; that is, $b_i > 0$ $\forall i$. There is a well-known one-one correspondence between sequences $(p_i)_0^n$ of monic orthogonal polynomials and nth order Jacobi matrices J. This correspondence is given by the rule that

$$p_j(t) = \det(t - J_j), \qquad j = 0, \dots, n$$

with J_j the left principal submatrix of order j of J. In terms of this correspondence, the abovementioned complementary sequence $(q_i)_0^n$ is given by

$$q_j(t) = \det(t - \bar{J}_j), \qquad j = 0, \dots, n,$$

where $\bar{J}_j$ the *right* principal submatrix of order j of J.

This led us to consider the following recovery problem, in which we denote by $J_{\setminus k}$ the principal submatrix of J obtained by deleting the kth row and column from J.

Given an integer k, $1 < k < n$, and the sequences $\lambda := (\lambda_i)_1^n$ and $\mu := (\mu_i)_1^{n-1}$, determine an nth order Jacobi matrix J that has $\lambda_1, \dots, \lambda_n$ as its eigenvalues and $\mu_1, \dots, \mu_{n-1}$ as the eigenvalues of its principal submatrix $J_{\setminus k}$.

The numerical solution of this problem for the cases $k = 1$ and $k = n$ was the subject of [BG] and, more recently, [GH]. These cases are also discussed in other publications, e.g., [GW], [Ha], and [Hoc]. Here we take the opportunity to discuss the remaining cases $k = 2, \dots, n-1$.

Existence of a solution to this problem can only be ensured under certain conditions. Assuming that $\lambda_1 < \cdots < \lambda_n$ and $\mu_1 \leqslant \cdots \leqslant \mu_{n-1}$, these conditions are

$$\lambda_i \leqslant \mu_i \leqslant \lambda_{i+1}, \qquad \text{all } i, \tag{0.3}$$

and

$$\lambda_i = \mu_i \quad \Leftrightarrow \quad \lambda_i = \mu_{i-1}. \tag{0.4}$$

We shall show that the recovery problem has a unique solution if the condition

$$\lambda_i < \mu_i < \lambda_{i+1}, \qquad i = 1, \dots, n-1, \tag{0.5}$$

holds and $k-1$ of the μ_i's have been chosen to make up the spectrum of the submatrix J_{k-1}. However, if $\mu_{i-1} = \lambda_i = \mu_i$ for one or more i, then [with the assumptions of (0.3) and (0.4)] the recovery problem has infinitely many solutions.

1. DISCRETE ORTHOGONALITY

We are given a set $X = \{x_1, \dots, x_n\}$ of n distinct real points, which we assume ordered, $x_1 < \cdots < x_n$, when convenient. We shall consider the discrete inner product

$$\langle f, g \rangle := \sum_{x \in X} f(x) g(x).$$

This means that we are only concerned with functions restricted to X, and therefore write

$$f \underset{X}{=} g$$

to mean that $f(x) = g(x)$ for all $x \in X$; this implies $f = g$ in the ordinary sense as long as $f, g \in \pi_{n-1}$. We also write $f \perp g$ when $\langle f, g \rangle = 0$.

Let

$$P := P_X := \prod_{x \in X} (\cdot - x).$$

Then

$$[x_1, \ldots, x_n] f = \sum_{i=1}^{n} \frac{f(x_i)}{\prod_{j \neq i} (x_i - x_j)} = \langle f, \frac{1}{P'} \rangle,$$

and so

$$\frac{1}{P'} \perp \pi_{n-2}. \tag{1.1}$$

This implies

LEMMA 1. $(\pi_{k-1})^{\perp} \underset{X}{=} \pi_{n-k-1}/P'$, $k = 1, \ldots, n$.

Proof. Both sides are linear spaces of dimension $n - k$, and the right side is obviously contained in the left, since for any $p \in \pi_{k-1}$ and $q \in \pi_{n-k-1}$, we have $pq \in \pi_{n-2}$ and so, by (1.1),

$$\langle p, \frac{q}{P'} \rangle = \langle pq, \frac{1}{P'} \rangle = 0. \qquad \blacksquare$$

Let $(p_j)_0^n$ be the sequence of monic orthogonal polynomials for the inner product $\langle \cdot, \cdot \rangle_w$, with

$$\langle f, g \rangle_w := \langle fw, g \rangle$$

and $w > 0$. Then Lemma 1 implies

COROLLARY. $p_j \underset{X}{=} q p_{n-1}$ *for some* $q \in \pi_{n-j-1}$.

Proof. Since $p_j w \perp \pi_{j-1}$, we have $p_j w \underset{X}{=} q/P'$ for some $q \in \pi_{n-j-1}$. In particular,

$$p_{n-1} w \underset{X}{=} \frac{c}{P'} \qquad \text{for some constant} \quad c \neq 0;$$

hence

$$p_j w \underset{X}{=} \frac{q}{p'} \underset{X}{=} \frac{q p_{n-1} w}{c},$$

from which the corollary follows. ■

REMARK. The fact that p_{n-1} doesn't vanish on X, i.e. $c \neq 0$, is quite evident here, since $p_{n-1}(x) = 0$ for some $x \in X$ would imply $p_{n-1} \underset{X}{=} 0$, which is impossible for a monic polynomial of degree $n-1$.

The corollary answers the question concerning discrete least squares and matching of divided differences raised in the introduction. Let $P_j f$ denote the weighted discrete least squares approximation to f from π_j, i.e.,

$$P_j f := \sum_{i \leqslant j} \frac{\langle fw, p_i \rangle}{\langle p_i w, p_i \rangle} p_i.$$

PROPOSITION 1. *Let $g \in \pi_j$. Then $g = P_j f$ iff*

$$[x_i, \dots, x_{i+n-j-1}] \frac{g}{p_{n-1}} = [x_i, \dots, x_{i+n-j-1}] \frac{f}{p_{n-1}}, \qquad \text{all } i,$$

i.e., for $i = 1, \dots, j+1$.

Proof. It is clear that $g = P_j f$ iff $(f-g)/p_{n-1} \in \operatorname{span}(p_i/p_{n-1} : i > j)$. By the Corollary to Lemma 1,

$$\frac{p_i}{p_{n-1}} \underset{X}{=} q \qquad \text{for some} \quad q \in \pi_{n-i-1}.$$

Hence the $n-j-1$ functions $(p_i/p_{n-1} : i = j+1, \dots, n-1)$ all lie in π_{n-j-2} (when considered as functions on X) and so, since they are linearly independent, must form a basis for π_{n-j-2}. Moreover, $h \in \pi_{n-1}$ is actually in π_{n-j-2} iff

$$[x_i, \dots, x_{i+n-j-1}] h = 0 \qquad \text{for} \quad i = 1, \dots, j+1.$$ ■

REMARK. Since, as we have just seen, $(p_i/p_{n-1})_{j+1}^{n-1}$ is a basis for π_{n-j-2} for all j, it follows that p_j/p_{n-1} must be of exact degree $n-j-1$, all i. This allows us to define q_{n-j-1} as the *monic* polynomial of degree $n-j-1$ for which

$$p_j \underset{X}{=} c_j q_{n-j-1} p_{n-1} \tag{1.2}$$

for some constant c_j.

2. THE COMPLEMENTARY SEQUENCE

We call the sequence $(q_i)_0^{n-1}$ of monic polynomials defined by (1.2) *complementary* to $(p_i)_0^{n-1}$. As one can immediately verify, the q_i's are also *orthogonal*, but with respect to a possibly different inner product; namely, the one with the weight

$$w^* := wp_{n-1}^2.$$

This makes it possible to state Proposition 1 in the following form.

PROPOSITION 2. *Let $P_j f$ ($Q_j f$) be the w-weighted (w^*-weighted) least squares approximation to f from π_j. Then*

$$f \underset{X}{=} P_j f + p_{n-1} Q_{n-j-2}\left(\frac{f}{p_{n-1}}\right). \tag{2.1}$$

Proof. From (1.2) and the definition of w^*, we have

$$\begin{aligned}\frac{f - P_j f}{p_{n-1}} &\underset{X}{=} \sum_{i>j} \frac{\langle fw, p_i\rangle}{\langle p_i w, p_i\rangle} \frac{p_i}{p_{n-1}} \\ &\underset{X}{=} \sum_{i>j} \frac{\langle (f/p_{n-1}) w^*, q_{n-i-1}\rangle}{\langle q_{n-i-1} w^*, q_{n-i-1}\rangle} q_{n-i-1} \\ &\underset{X}{=} \quad Q_{n-j-2}(f/p_{n-1}).\end{aligned}$$

■

The particular connection between the two sequences $(p_i)_0^{n-1}$, $(q_i)_0^{n-1}$ has been explored before, in [BG], where the following is shown.

Fact. *Let J in* (0.2) *be the Jacobi matrix for* $(p_i)_0^n$, *i.e.*,

$$(t-J)(1,\ldots,j)=p_j(t), \qquad \textit{all } j. \tag{2.2}$$

Then X is the spectrum of J, and

$$(t-J)(j+1,\ldots,n)=q_{n-j}(t), \qquad \textit{all } j. \tag{2.3}$$

Thus, our defining equation (1.2) for q_{n-j-1} can also be thought of as a determinant identity. In fact, starting with (2.2) and (2.3) as *definitions* and using Laplace's expansion by minors, one gets

$$p_i q_{n-i} - b_i^2 p_{i-1} q_{n-i-1} = p_n = P, \tag{2.4}$$

which can already be found in [Hou, p. 48]. Indeed, more explicitly than (1.2),

$$\left(b_{n-1}\cdots b_{j+1}\right)^2 p_j \underset{X}{=} q_{n-j-1} p_{n-1}. \tag{2.5}$$

In any case, it follows from the Fact that

$$r := p_{k-1} q_{n-k} = (\cdot - J)(1,\ldots,k-1,k+1,\ldots,n),$$

that is, $r(t)$ is the $(n-1)$st order principal minor of $t-J$ obtained by omitting the kth row and column. The results of [BG] are concerned with reconstructing J from $p_n = P$ and r for $k=1$ or $k=n$. We prepare now to consider this problem for $k=2,\ldots,n-1$.

This requires a precise description of the possible zero set of such a minor. We write

$$p := p_{k-1}, \qquad q := q_{n-k}$$

for short, and derive the necessary information directly from the defining identity (1.2), i.e., from

$$p \underset{X}{=} c q p_{n-1}, \tag{2.6}$$

together with the facts that $p \in \pi_{k-1}$, $q \in \pi_{n-k}$, $c \neq 0$.

Since p_{n-1} does not vanish on X, (2.6) implies that

$$p(x_i)=0 \quad \text{iff} \quad q(x_i)=0. \tag{2.7}$$

Now define $Z_r(a)$ to be the multiplicity with which a is a zero of $r := pq$, i.e.,

$$Z_r(a) := \min\{j : r^{(j)}(a) \neq 0\}.$$

Further, for any interval $[a,b]$ define

$$Z_r[a,b] := \frac{Z_r(a)+Z_r(b)}{2} + \sum_{a<t<b} Z_r(t).$$

Then

$$Z_r[a,b] = Z_r[a,t] + Z_r[t,b] \qquad \text{for} \quad a<t<b.$$

THEOREM 1. *If* $r = p_{k-1}q_{n-k}$, *then* $Z_r[x_i, x_{i+1}] = 1$, *all* i.

Proof. We first prove that $Z_r[x_i, x_{i+1}] \geqslant 1$. Indeed, if $r(a)=0$ for $a=x_i$ or $a=x_{i+1}$, then also $r'(a)=0$ by (2.7); hence $Z_r(a) \geqslant 2$ in this case. Otherwise $r(a) \neq 0$ for $a = x_i$ and x_{i+1}; hence $r(x_i)r(x_{i+1}) < 0$, since $r \underset{X}{=} cq^2 p_{n-1}$, and therefore $Z_r(t) \geqslant 1$ for some $x_i < t < x_{i+1}$.

This implies that

$$n-1 \leqslant \sum Z_r[x_i, x_{i+1}] = Z_r[x_1, x_n] \leqslant Z_r(\mathbf{R}) \leqslant n-1;$$

hence equality must hold throughout. ∎

The proof shows that, in fact, all the zeros of r lie in the *open* interval (x_1, x_n). The theorem implies that each interval $[x_i, x_{i+1}]$ contains a zero of r. If this is an interior zero, then it must be a simple zero and the only zero there, of either p or q, and we call $[x_i, x_{i+1}]$ accordingly a p-interval or a q-interval. Else, it is a boundary zero. But then it must be a zero of both p and q, by (2.7); hence it is a double zero of r, and again r cannot vanish elsewhere in $[x_i, x_{i+1}]$. In this case, we call $[x_i, x_{i+1}]$ a pq-interval. Since this zero cannot be x_1 or x_n, it follows that pq-intervals come in pairs, with the zero their common end point.

This implies that $p_{k-1} = P_U$ and $q_{n-k} = P_V$, with the zero sets U and V satisfying the following conditions:

$$U, V \subseteq (x_1, x_n), \tag{2.8i}$$

$$\#U = k-1, \qquad \#V = n-k, \tag{2.8ii}$$

and for each i,

$$\#(U \cup V) \cap [x_i, x_{i+1}] = 1$$

and

$$(U \cap V) \cap [x_i, x_{i+1}] = (U \cup V) \cap \{x_i, x_{i+1}\}. \tag{2.8iii}$$

With this, we have established half of the following.

THEOREM 2. *Given U and V, there exist weights w such that $p_{k-1} = P_U$ and $q_{n-k} = P_V$ iff U, V satisfy* (2.8).

Proof. We show how to construct the requisite weight w from U and V. Let $p := P_U$, $q := P_V$. Guided by Lemma 1, we define

$$w_j := \begin{cases} \dfrac{q}{pP'}(x_j), & x_j \notin U \\ \text{positive} & \text{otherwise.} \end{cases} \tag{2.9}$$

We claim that $w_j > 0$, all j, and prove this by induction on j. For $j = n$, we have $x_n \notin U \cup V$ by (2.8i), and both q and p are monic with all zeros to the left of x_n; hence

$$\frac{q}{p}(x_n) > 0,$$

while also $P'(x_n) > 0$. Therefore $w_n > 0$. Assuming now that $w_{j+1}, w_{j+2}, \ldots,$ are known to be positive, consider w_j. If $x_j \in U$, then $w_j > 0$ by the definition. Otherwise $x_j \notin U$, and there are two cases:

If $x_{j+1} \notin U$, then, from (2.8iii), (x_j, x_{j+1}) contains exactly one point from $U \cup V$ and none from $U \cap V$; hence q/p changes sign across (x_j, x_{j+1}) and does not vanish at x_j, x_{j+1}. Since P' has the same property, we get $w_j w_{j+1} > 0$; hence $w_j > 0$.

If $x_{j+1} \in U$, then $j+1 < n$ by (2.8i) and $x_{j+1} \in V$, $x_{j+2} \notin U$ by (2.8iii). Hence both p and q change sign across (x_j, x_{j+2}), viz. at x_{j+1}, and so q/p does not change sign across (x_j, x_{j+2}). Since also $P'(x_j)P'(x_{j+2}) > 0$, we get $w_j w_{j+2} > 0$; hence $w_j > 0$.

Since $pw \underset{X}{=} q/P'$ by (2.9), it now follows from Lemma 1 that $pw \perp \pi_{k-2}$. Since p is also monic of degree $k-1$, this proves that p is the $(k-1)$st monic orthogonal polynomial for the scalar product $\langle \cdot, \cdot \rangle_w$. Further,

$$pw \underset{X}{=} \frac{q}{P'} \underset{X}{=} \frac{q p_{n-1} w}{c}$$

for some constant c. Hence, by (1.2), $q = q_{n-k}$. ∎

We have in hand all the information required to answer a related question.

Corollary. *For any U there exists a sequence $\{p_i\}_0^n$ of monic orthogonal polynomials such that $P_U = p_{k-1}$ and $P_X = p_n$ iff*

$$U \subseteq (x_1, x_n), \tag{2.10i}$$

$$\#U = k-1 \tag{2.10ii}$$

$$\#U \cap [x_i, x_{i+1}] \leqslant 1, \qquad \forall i; \tag{2.10iii}$$

$$\#X \cap U \leqslant n-k. \tag{2.10iv}$$

Proof. Under these conditions,

$$\sum \#U \cap [x_i, x_{i+1}] = k-1+\#X \cap U;$$

hence there are exactly $n-1-(k-1+\#X \cap U) = n-k-\#X \cap U$ intervals $[x_i, x_{i+1}]$ entirely free of U, and this number is nonnegative by (2.10iv). We can therefore obtain a V such that U, V satisfy (2.8) by adjoining to $X \cap U$ one point from the interior of each U-free interval $[x_i, x_{i+1}]$. ∎

Remark. We recognize in (2.10iii) the well-known necessary condition (see, e.g. [S, Theorem 3.3.3]) that any two points of U be separated by a point in X. Thus only (2.10iv) is not mentioned in standard texts.

3. RECOVERY OF A JACOBI MATRIX FROM SPECTRAL INFORMATION

Suppose now that we are given the spectrum $\lambda_1,\ldots,\lambda_n$ of a Jacobi matrix J along with the spectrum $\mu_1,\ldots,\mu_{n-1}$ of its $n-1$ order principal submatrix $J_{\setminus k}$, and wish to reconstruct J from this information, by choosing an appropriate weighted discrete scalar product $\langle\cdot,\cdot\rangle_w$ and generating the entries of J as the coefficients in the three-term recurrence relation for the corresponding sequence $(p_i)_0^n$ of monic orthogonal polynomials. We set $X=(\lambda_1,\ldots,\lambda_n)$, of course. Further, it must be possible to split $\mu_1,\ldots,\mu_{n-1}$ into two sets U and V satisfying (2.8). Since we assume that $1<k<n$, this can be done in *many* ways if it can be done at all. Assuming that $\mu_1 \leqslant \cdots \leqslant \mu_{n-1}$, one checks that it can be done at all provided there are no more than $\min\{k-1, n-k\}$ doublets in the sequence μ, and μ_i is the one and only point of μ in $[x_i, x_{i+1}]$, all i, with the convention that any doublet $\mu_j = d = \mu_{j+1}$ is split into $\mu_j := d^-$ and $\mu_{j+1} := d^+$. Once we have split $\mu_1,\ldots,\mu_{n-1}$ into suitable U and V, taking care that, from any doublet, one member gets into U and the other into V, the Jacobi matrix is uniquely determined in case there are no doublets in μ. If there are m doublets, then there is an m-parameter family of Jacobi matrices, parametrized by the corresponding free choice of m of the weights. One can obtain all of these Jacobi matrices as limits of Jacobi matrices corresponding to nearby *strictly* increasing μ, as certain neighboring μ_i's, one from U and the other from V, coalesce.

REMARK concerning computations. Use of the weights (2.9) produces the entries of J from top to bottom. It follows that using instead the weight w^* given by

$$w_j^* := \begin{cases} \dfrac{p}{qP'}(x_j), & x_j \notin U, \\ \text{positive} & \text{otherwise} \end{cases}$$

produces the entries of J from bottom to top. As in the case $k=n$ discussed in [BG], one would prefer to work with w in case $k-1 \leqslant n-k$ and with w^* otherwise, since this will more nearly balance numerator and denominator.

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