ORTHOGONAL MATRIX POLYNOMIALS AND HIGHER ORDER RECURRENCE RELATIONS

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Abstract. It is well-known that orthogonal polynomials on the real line satisfy a three-term recurrence relation and conversely every system of polynomials satisfying a three-term recurrence relation is orthogonal with respect to some positive Borel measure on the real line. In this paper we extend this result and show that every system of polynomials satisfying some $(2N + 1)$-term recurrence relation can be expressed in terms of orthonormal matrix polynomials for which the coefficients are $N \times N$ matrices. We apply this result to polynomials orthogonal with respect to a discrete Sobolev inner product and other inner products in the linear space of polynomials. As an application we give a short proof of Krein’s characterization of orthogonal polynomials with a spectrum having a finite number of accumulation points.

1. Introduction

A sequence of orthonormal polynomials $p_n(x) \ (n = 0, 1, 2, \ldots)$ on the real line, orthonormal with some probability measure $\mu$, always satisfies a three-term recurrence relation

\begin{equation}
xp_n(x) = a_{n+1}p_{n+1}(x) + b_n p_n(x) + a_n p_{n-1}(x),
\end{equation}

with initial conditions $p_{-1}(x) = 0$ and $p_0(x) = 1$. The recurrence coefficients are given by

\[ a_n = \int xp_{n-1}(x)p_n(x) \, d\mu(x) > 0, \quad b_n = \int xp_n^2(x) \, d\mu(x) \in \mathbb{R}. \]

The converse is also true: a system of polynomials satisfying a three-term recurrence relation (1.1) with $a_{n+1} > 0$ and $b_n \in \mathbb{R} \ (n = 0, 1, 2, \ldots)$ is always a system of orthonormal polynomials with respect to some probability measure $\mu$ on the real line. This converse result was given by Favard in 1935 [10] but was known earlier and appears already in the books by Stone [21, Theorem 10.27 on pp. 545–546],

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Perron [18, §36, Satz 4.6/4.7] and Wintner [22, §32 and §87] who attributes the case of finite support to E. Heine [12, §108]. In an elementary form (lacking the Riesz representation theorem) the result is in Stieltjes' 1894 work [20, §11] and apparently the result was already known by Chebyshev [5] when the support of the measure $\mu$ is finite.

The importance of Favard's theorem is that orthogonal polynomials and polynomials satisfying a three-term recurrence relation are the same thing. Properties regarding zeros (real and simple zeros, interlacing of zeros) and positivity of connection coefficients can thus be studied from two points of view: on one hand using the orthogonality, on the other hand using the recurrence relation.

Favard's theorem can also be proved for orthogonal matrix polynomials. Orthogonal matrix polynomials on the real line have been considered in detail by M.G. Krein [13]. See also the book by Berezanskiǐ [4] and more recent papers by Aptekarev and Nikishin [1], Geronimo [11], and Sinap and Van Assche [19].

Consider matrix polynomials satisfying the three-term recurrence relation

$$xp_k(x) = D_{k+1}p_{k+1}(x) + E_kp_k(x) + D_k^*p_{k-1}(x),$$

with $P_0(x) = I$ and $P_{-1}(x) = 0$, where $P_k(x)$ are matrix polynomials with coefficients in $\mathbb{C}^{N \times N}$ and the recurrence coefficients $D_{k+1}, E_k$ are also $N \times N$ matrices for which $E_k^* = E_k$ and $\det D_k \neq 0$. By using spectral theory Aptekarev and Nikishin [1] show that the polynomials $P_n(x)$ $(n = 0, 1, 2, \ldots)$ are orthonormal with respect to some Hermitian matrix of measures $M = (\mu_{k,l})_{k,l=1}^N$ which is positive definite:

$$\int P_n(x) dM(x) P_m^*(x) = \delta_{m,n} I.$$ 

Recently one of us studied polynomials $p_n(x)$ satisfying a $(2N + 1)$-term recurrence relation

$$h(x)p_n(x) = c_{n,0}p_n(x) + \sum_{k=1}^N (c_{n,k}p_{n-k}(x) + c_{n+k,k}p_{n+k}(x)),$$

where $h$ is a polynomial of degree $N$ and $c_{n,k}$ $(n = 0, 1, 2, \ldots)$ are real sequences for $k = 0, 1, \ldots, N$ with $c_{n,N} \neq 0$. From [7] we get, after straightforward reformulation, that a sequence of polynomials satisfies a $(2N + 1)$-term recurrence relation if and only if the following orthogonality condition holds: there exists a $N \times N$ matrix of measures $\mu = (\mu_{k,l})_{k,l=0}^{N-1}$ such that the bilinear form

$$B_\mu(p,q) = \sum_{k,l=0}^{N-1} \int R_{h,N,k}(p)R_{h,N,l}(q) d\mu_{k,l},$$

where

$$R_{h,N,k}(x) = \sum_{n=0}^m a_{k,n}x^n \quad \text{if} \quad p(x) = \sum_{k=0}^{N-1} \sum_{n=0}^m a_{k,n}x^k h^n(x)$$

is an inner product on the linear space of polynomials $\mathbb{P}$ and $(p_n)_n$ is the sequence of orthonormal polynomials with respect to $B_\mu$. In [8] this is improved showing that the matrix of measures $\mu$ can be taken to be positive definite.
In Section 2 we will show that polynomials satisfying a higher order recurrence relation of the form (1.3) (but with complex coefficients) are closely related to matrix polynomials satisfying a three-term recurrence relation and that Favard’s theorem for matrix polynomials and Favard’s theorem for polynomials satisfying a higher order recurrence relation are the same.

In Section 3 we show how discrete Sobolev orthogonal polynomials and some new orthogonal polynomials with respect to an inner product of the form

$$\langle f, g \rangle = \int f(x)g(x) \, d\mu(x) + \left( \sum_{k=1}^{N} a_k f(c_k) \right) \left( \sum_{k=1}^{N} a_k g(c_k) \right), \quad a_k, c_k \in \mathbb{R}$$

are related to orthogonal matrix polynomials and we explicitly give the orthogonality matrix of measures $\mathbf{M}$ in terms of the parameters in the inner product. The advantage of working with the matrix polynomials is that the orthogonality conditions no longer require the evaluation of a function and its derivatives in various points. Finally, in Section 4 we show how Krein’s theorem regarding orthogonal polynomials with a spectrum with finitely many accumulation points follows easily by this correspondence between higher order recurrence relations and orthogonal matrix polynomials on the real line.

The connection between matrix polynomials and scalar polynomials obtained in the present paper shows some analogy with the connection between orthogonal polynomials on a lemniscate and orthogonal polynomials on the unit circle, as given by Marcellán and Rodríguez [15] and the connection between orthogonal polynomials on an algebraic harmonic curve and orthogonal matrix polynomials on the real line, as given by Marcellán and Sansigre [17]. In fact the particular choice of basis in the linear space of polynomials that we use in Sections 2 and 3 is the same as the basis used in [15] and [17], but the polynomial $h(x)$ in the present paper is connected with the recurrence relation, whereas in [15] this polynomial describes the lemniscate and in [17] it describes the algebraic harmonic curve.

### 2. Recurrence Relation and Matrix Polynomials

In order to establish the main theorem we need to consider the operators $R_{h,N,k}$ defined in the introduction of this paper (see (1.5)). For the sake of simplicity we start by considering the case $h(x) = x^N$. Then, we denote the operators by $R_{N,m}$ and it is not hard to see that they are defined by

$$R_{N,m}(p)(x) = \sum_n p^{(nN+m)}(0) (nN+m)! x^n,$$

i.e., the operator $R_{N,m}$ takes from $p$ just those powers with remainder $m$ modulo $N$ and then, removes $x^m$ and changes $x^N$ to $x$. Thus, we have

$$p(x) = R_{N,0}(p)(x^N) + xR_{N,1}(p)(x^N) + \cdots + x^{N-1}R_{N,N-1}(p)(x^N).$$

For example, when $N = 3$ and $p(x) = 6x^5 + 5x^4 + 4x^3 + 3x^2 + 2x + 1$ we have $R_{3,0}(p)(x) = 4x + 1$, $R_{3,1}(p)(x) = 5x + 2$, $R_{3,2}(p)(x) = 6x + 3$. For $N = 2$ this corresponds to taking the odd ($R_{2,1}$) and even ($R_{2,0}$) parts of the polynomial $p$.

Now, we are ready to establish the following
Theorem. Suppose \( p_n(x) \) (\( n = 0, 1, 2, \ldots \)) is a sequence of polynomials satisfying the following \((2N + 1)\)-term recurrence relation

\[
(2.1) \quad x^N p_n(x) = c_{n,0} p_n(x) + \sum_{k=1}^{N} (c_{n,k} p_{n-k}(x) + c_{n+k,k} p_{n+k}(x)),
\]

where \( c_{n,0} \) (\( n = 0, 1, 2, \ldots \)) is a real sequence and \( c_{n,k} \) (\( n = 0, 1, 2, \ldots \)) are complex sequences for \( k = 1, \ldots, N \) with \( c_{n,k} \neq 0 \) for every \( n \) and with the initial conditions \( p_k(x) = 0 \) for \( k < 0 \) and \( p_k \) given polynomials of degree \( k \), for \( k = 0, \ldots, N - 1 \).

We define the sequence of matrix polynomials \((P_n)_n\) by

\[
P_n(x) = \begin{pmatrix}
R_{N,0}(p_{nN})(x) & \cdots & R_{N,N-1}(p_{nN})(x) \\
R_{N,0}(p_{nN+1})(x) & \cdots & R_{N,N-1}(p_{nN+1})(x) \\
\vdots & \ddots & \vdots \\
R_{N,0}(p_{nN+N-1})(x) & \cdots & R_{N,N-1}(p_{nN+N-1})(x)
\end{pmatrix},
\]

Then this sequence of matrix polynomials is orthonormal on the real line with respect to a positive definite matrix of measures and satisfies a matrix three-term recurrence relation. Conversely, suppose \( P_n = (P_{n,m,j})_{n,j=0}^{N-1} \) is a sequence of orthonormal matrix polynomials or equivalently satisfying a matrix three-term recurrence relation (without loss of generality we can assume the leading coefficient of \( P_n \) to be a lower triangular matrix), then the scalar polynomials defined by

\[
(2.2) \quad p_{nN+m}(x) = \sum_{j=0}^{N-1} x^j P_{n,m,j}(x^N), \quad (n \in \mathbb{N}, 0 \leq m \leq N - 1),
\]

satisfy a \((2N + 1)\)-term recurrence relation of the form (2.1).

Proof. The equivalence between \((p_n)_n\) satisfying a \((2N+1)\)-term recurrence relation and \((P_n)_n\) being a sequence of matrix orthonormal polynomials is a consequence of the definition of the \( P_n \) from the \( p_k \) (or conversely, the \( p_k \) from the \( P_n \)) and the orthogonality condition (1.4).

Let us show that the matrix polynomials \((P_n)_n\) satisfy a matrix three-term recurrence relation, giving explicitly the matrix coefficients which appear in this recurrence formula. To do that, we consider the \( N \)-Jacobi matrix \( J \) associated to \((p_n)_n\), which is the \((2N + 1)\)-banded infinite Hermitian matrix defined by putting the sequences \((c_{n,l})_n\) which appear in the recurrence relation on the diagonals of the matrix \( J \), i.e., we define the matrix \( J = (j_{n,m})_{n,m \in \mathbb{N}} \) by

\[
j_{n,m} = \begin{cases}
    c_{n,|n-m|} & \text{if } 0 \leq n - m \leq N, \\
    c_{m,|n-m|} & \text{if } 0 \leq m - n \leq N, \\
    0 & \text{if } |n-m| > N.
\end{cases}
\]

Now, we split up this \( N \)-Jacobi matrix in blocks of dimension \( N \times N \), and then we get the \( N \times N \) matrices \( E_n \) and \( D_n \) defined by

\[
(E_n)_{i,l} = j_{nN+i,nN+l} = \begin{cases}
    c_{nN+i,|i-l|} & \text{if } i \geq l, \\
    c_{nN+i,|i-l|} & \text{if } i < l. 
\end{cases} \quad (n \geq 0, \quad i, l = 0, 1, \ldots, N - 1).
\]
and

\[
(D_n)_{i,l} = \begin{cases} 
0 & \text{if } i < l, \\
\delta_{i} & \text{if } i \geq l,
\end{cases}
\]

\[
= \begin{cases} 
0 & \text{if } i < l, \\
c_{nN+l,N+l-i} & \text{if } i \geq l,
\end{cases}
\]

i.e.,

\[
J = \begin{pmatrix}
E_0 & D_1 \\
D_1^* & E_1 & D_2 \\
& & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & \ddots & \ddots \\
\end{pmatrix}
\]

with

\[
D_n = \begin{pmatrix}
c_{nN,N} & 0 & 0 & \cdots & 0 \\
c_{nN,N-1} & c_{nN+1,N} & 0 & \cdots & 0 \\
c_{nN,N-2} & c_{nN+1,N-1} & c_{nN+2,N} & \cdots & 0 \\
& \ddots & \ddots & \ddots & \ddots \\
c_{nN,1} & c_{nN+1,2} & c_{nN+2,3} & \cdots & c_{nN+N-1,N}
\end{pmatrix},
\]

and

\[
E_n = \begin{pmatrix}
c_{nN,0} & c_{nN+1,1} & c_{nN+2,2} & \cdots & c_{nN+N-1,N-1} \\
c_{nN+1,1} & c_{nN+1,0} & c_{nN+2,1} & \cdots & c_{nN+N-1,N-2} \\
c_{nN+2,2} & c_{nN+2,1} & c_{nN+2,0} & \cdots & c_{nN+N-1,N-3} \\
& \ddots & \ddots & \ddots & \ddots \\
c_{nN+N-1,N-1} & c_{nN+N-1,N-2} & c_{nN+N-1,N-3} & \cdots & c_{nN+N-1,0}
\end{pmatrix}
\]

Then \(E_n\) is an Hermitian matrix, and the conditions \(c_{n,N} \neq 0\) shows that \(D_n\) is a lower triangular matrix with \(\det D_n \neq 0\).

If we compute the following expression

\[
(2.3) \quad D_{n+1}P_{n+1}(x) + E_nP_n(x) + D_n^*P_{n-1}(x)
\]

we find that the entry \((k, m) (0 \leq k, m \leq N - 1)\) of this matrix is equal to

\[
\sum_{j=0}^{k-1} c_{nN+j,N+j-k}R_{N,m}(p_{(n+1)N+j})(x)
\]

\[
+ \sum_{j=0}^{k-1} c_{nN+k+[k-j]}R_{N,m}(p_{nN+j})(x) + \sum_{j=k}^{N-1} c_{nN+j,[k-j]}R_{N,m}(p_{nN+j})(x)
\]

\[
+ \sum_{j=k}^{N-1} c_{nN+k,N+k-j}R_{N,m}(p_{(n-1)N+j})(x),
\]

that is,

\[
(2.4) \quad c_{nN+k,0}R_{N,m}(p_{nN+k})(x)
\]

\[
+ \sum_{j=0}^{N} (c_{nN+k,l-j}R_{N,m}(p_{nN+k-l})(x) + c_{nN+k+l,l}R_{N,m}(p_{nN+k+l})(x)).
\]
But from the \((2N+1)\)-term recurrence relation which the polynomials \((p_n)_n\) satisfy, it follows that the sequence of polynomials \((R_{N,i}(p_n))_n\) \((i = 0, \ldots, N - 1)\) satisfies the following recurrence formula

\[
xR_{N,i}(p_n)(x) = c_{n,0}R_{N,i}(p_n)(x) + \sum_{l=1}^{N} (c_{n,l}R_{N,i}(p_{n-l})(x) + c_{n+l,l}R_{N,i}(p_{n+l})(x))
\]

and so (2.4) is equal to \(xR_{N,m}(p_{nN+k})(x)\). Hence (2.3) is equal to \(xP_n(x)\) and we have proved that the sequence of matrix polynomials satisfies the matrix three-term recurrence relation

\[
xP_n(x) = D_{n+1}P_{n+1}(x) + E_nP_n(x) + D^*_nP_{n-1}(x).
\]

Note that the matrix polynomials obtained in this way always have a leading coefficient which is a lower triangular matrix and also the matrices \(D_n\) which appear in the recurrence formula are lower triangular.

To prove the converse, suppose \((P_n)_n\) is a sequence of matrix polynomials satisfying the recurrence formula

\[
xP_n(x) = D_{n+1}P_{n+1}(x) + E_nP_n(x) + D^*_nP_{n-1}(x),
\]

where \(\det D_n \neq 0\). First, we prove that we can assume both the leading coefficients of \(P_n\) and the matrices \(D_n\) to be lower triangular matrices, which is necessary since otherwise the scalar polynomials \(p_n\) defined by (2.2) could have degree different from \(n\). Orthonormal matrix polynomials for a given orthogonality measure \(M\) are only determined up to a unitary factor \(U_n\) in the sense that \(U_nP_n(x)\) is also orthonormal with respect to the measure \(M\) whenever \(U_nU_n^* = I\). If \(Q_n(x)\) is a sequence of orthonormal matrix polynomials satisfying

\[
xQ_n(x) = A_{n+1}Q_{n+1}(x) + B_nQ_n(x) + A_n^*Q_{n-1}(x),
\]

then the polynomials \(P_n(x) = U_nQ_n(x)\), with \(U_nU_n^* = I\), satisfy

\[
xP_n(x) = U_nA_{n+1}U_{n+1}^*P_{n+1}(x) + U_nB_nU_n^*P_n(x) + U_nA_n^*U_{n-1}^*P_{n-1}(x).
\]

If the non-singular matrices \(A_n\) are not lower triangular, one can always find unitary matrices \(U_n\) such that

\[
D_n = U_{n-1}A_nU_n^*
\]

are lower triangular matrices. These unitary matrices are given recursively as follows. First we choose a unitary matrix \(U_0\) such that \(U_0Q_0 = P_0\) is lower triangular. Next we observe that the matrix \(U_0A_1\) can always be factorized as \(U_0A_1 = D_1U_1\), where \(U_1\) is a unitary matrix and \(D_1\) is lower triangular (QR-factorization of Francis and Kublanovskaja). With this choice of \(U_1\) we thus have \(D_1 = U_0A_1U_1^*\). In general, if \(U_0, U_1, \ldots, U_{n-1}\) have been obtained, then we apply the QR-factorization to \(U_{n-1}A_n\) to find a unitary matrix \(U_n\) with \(U_{n-1}A_n = D_nU_n\), with \(D_n\) lower triangular. Therefore any system of orthonormal matrix polynomials can be transformed to a system of orthonormal matrix polynomials with leading coefficients which are lower triangular.
Now, since we can assume the leading coefficient of $P_n$ to be lower triangular with non-vanishing determinant, the sequence of scalar polynomials $(p_n)_n$ defined by (2.2) are such that $\text{dgr}(p_n) = n$. And proceeding as before, it is no hard to prove that they satisfy a $(2N + 1)$-term recurrence relation like (2.1). The coefficients in this recurrence formula can be obtained from the matrices $D_n, E_n$. □

For the general case of a $(2N + 1)$-term recurrence relation defined by a polynomial $h$ of degree $N$

\[
h(x)p_n(x) = c_{n,0}p_n(x) + \sum_{k=1}^{N} (c_{n,k}p_{n-k}(x) + c_{n+k,k}p_{n+k}(x)),
\]

the theorem works again if we change the operators $R_{N,m}$ to $R_{h,N,m}$ ($m = 0, \cdots, N - 1$) (see (1.5)) in the definition of the matrix polynomials $P_n$ from the scalar polynomials $p_n$. Thus, in the definition of the operators $R_{h,N,m}$, instead of using the basis of monomials $\{1, x, x^2, x^3, \ldots\}$ to span the linear space of polynomials, we will use the basis

\[
\{1, x, \ldots, x^{N-1}, h(x), xh(x), \ldots, x^{N-1}h(x), h^2(x), xh^2(x), \ldots\}
\]

\[
= \{x^n h^m(x) : n = 0, 1, \ldots, N - 1, m = 0, 1, 2, \ldots\}.
\]

A polynomial $p$ of degree $nN + m$ ($0 \leq m < N$) can then be expanded in this basis as

\[
p(x) = \sum_{i=0}^{n} \sum_{j=0}^{N-1} a_{i,j} x^j h^i(x).
\]

Now, the operator $R_{h,N,j}$ takes from $p$ just those terms of the form $a_{i,j} x^j h^i(x)$ and then, removes the common factor $x^j$ and changes $h(x)$ to $x$.

Conversely, since now we have

\[
p(x) = R_{h,N,0}(p)(h(x)) + x R_{h,N,1}(h(x)) + \cdots + x^{N-1} R_{h,N,N-1}(p)(h(x))
\]

we change (2.2) in the theorem to

\[
p_{nN+m}(x) = \sum_{j=0}^{N-1} x^j P_{n,m,j}(h(x)), \quad (n \in \mathbb{N}, 0 \leq m \leq N - 1)
\]

in the definition of the scalar polynomials $p_n$ from the matrix polynomials $P_n$.

3. Examples

3.1 Discrete Sobolev orthogonal polynomials.

An important class of polynomials satisfying a higher order recurrence relation is obtained by taking polynomials orthogonal with respect to an inner product of (discrete) Sobolev type

\[
\langle f, g \rangle = \int f(x)g(x) \, d\mu(x) + \sum_{k=1}^{N} \lambda_k f^{(s_k)}(c_k)q^{(s_k)}(c_k),
\]

where $\mu$ is a measure with finite moments.
where $\lambda_k$ are positive real numbers and $c_k$ are real numbers (which are allowed to coincide). For a discrete Sobolev inner product

$$\langle f, g \rangle = \int f(x)g(x) \, d\mu(x) + \lambda f^{(r)}(c)g^{(r)}(c)$$

it was shown by Marcellán and Ronveaux [16] that the corresponding monic orthogonal polynomials $q_n(x)$ satisfy a $(2r + 3)$-term recurrence relation

$$(x - c)^{r+1}q_n(x) = \sum_{j=n-r-1}^{n+r+1} \gamma_{n,j} q_j(x).$$

The orthonormal polynomials then satisfy a recurrence relation of the form (1.3) with $h(x) = (x - c)^{r+1}$ and thus these polynomials are also orthogonal with respect to a positive definite matrix of measures. Evans et al. [9] consider weighted Sobolev inner products

$$\langle f, g \rangle = \sum_{k=0}^{N} \int f^{(k)}(x)g^{(k)}(x) \, d\mu_k(x),$$

and show that the existence of a polynomial $h$ for which

$$(3.1) \quad \langle hp, q \rangle = \langle p, hq \rangle$$

for all polynomials $p, q$ implies that the measures $\mu_k$ $(1 \leq k \leq N)$ are necessarily discrete with support at the zeros of $h$ and that the orthonormal polynomials satisfy a $(2N + 1)$-term recurrence relation of the form (1.3), where $N$ is the degree of the minimal polynomial $h$ for which (3.1) holds. It follows that polynomials which are orthonormal with respect to a discrete Sobolev inner product correspond to matrix polynomials orthonormal with respect to a positive definite matrix of measures.

Consider the discrete Sobolev inner product

$$(3.2) \quad \langle p, q \rangle = \int p(x)q(x) \, d\mu(x) + \sum_{i=1}^{M} \sum_{j=1}^{M_i} \lambda_{i,j} p^{(j)}(c_i)q^{(j)}(c_i),$$

where $p, q$ are polynomials, $\lambda_{i,j} \geq 0$ and $N = M + \sum_{i=1}^{M} M_i$. Here derivatives are taken at $M$ points $c_i \in \mathbb{R}$ and at the point $c_i$ the highest derivative is of order $M_i$. Introduce the polynomial

$$h(x) = \prod_{i=1}^{M} (x - c_i)^{M_i+1},$$

then $h$ is of degree $N$ and has its zeros at the points $c_i$ where the derivatives of the inner product are evaluated. Instead of using the basis of monomials $\{1, x, x^2, x^3, \ldots \}$ to span the linear space of polynomials, we will use the basis

$$(3.3) \quad \{1, x, \ldots, x^{N-1}, h(x), xh(x), \ldots, x^{N-1}h(x), h^2(x), xh^2(x), \ldots \} = \{x^n h^m(x) : n = 0, 1, \ldots, N-1, m = 0, 1, 2, \ldots \}.$$
A polynomial $p$ of degree $Nk + l$ ($0 \leq l < N$) can then be expanded in this basis as

$$p(x) = \sum_{n=0}^{N-1} \sum_{m=0}^{k} a_{n,m} x^n h^m(x),$$

where $a_{n,k} = 0$ whenever $n > l$. Taking the terms in $x^n$ together and putting

$$R_{h,N,n}(p)(x) = \sum_{m=0}^{k} a_{n,m} x^m,$$

then for $0 \leq n < N$ each polynomial $R_{h,N,n}(p)$ has degree at most $k$ (for $n > l$ the degree is less than $k$) and

$$p(x) = \sum_{n=0}^{N-1} x^n R_{h,N,n}(p)(h(x)).$$

The polynomial $p$ is thus equivalent (modulo $h$) with the vector polynomial given by $(R_{h,N,0}(p), R_{h,N,1}(p), \ldots, R_{h,N,N-1}(p))$ and we will write

$$p \equiv (R_{h,N,0}(p), R_{h,N,1}(p), \ldots, R_{h,N,N-1}(p)).$$

Observe again that in case $h(x) = x^2$ this amounts to the decomposition of a polynomial $p$ into its odd and even parts.

For the $j$th derivative of $p$ we then find, using Leibnitz’ rule for the derivative of a product,

$$p^{(j)}(x) = \sum_{n=j}^{N-1} \sum_{k=0}^{j} \binom{j}{k} n(n-1) \cdots (n-k+1) x^{n-k} \frac{d^{j-k}}{dx^{j-k}} R_{h,N,n}(p)(h(x)).$$

The derivative of the composite function $R_{h,N,n}(p)(h(x))$ can be evaluated using the formula of Faa di Bruno, giving

$$\frac{d^m}{dx^m} R_{h,N,n}(p)(h(x)) = \sum_{i=0}^{m} \frac{d^i}{dh^i} R_{h,N,n}(p)(h) \sum_{a_1, \ldots, a_m} \binom{m}{a_1, a_2, \ldots, a_m} \left( \frac{h'(x)}{1!} \right)^{a_1} \cdots \left( \frac{h^{(m)}(x)}{m!} \right)^{a_m},$$

where $a_i$ are non-negative integers satisfying $a_1 + a_2 + \cdots + a_m = i$ and $a_1 + 2a_2 + \cdots + ma_m = m$. If $m \leq M_i$ and if we evaluate this expression at $c_i$ then due to the fact that $h'(c_i) = \cdots = h^{(m)}(c_i) = 0$ we see that

$$\frac{d^m}{dx^m} R_{h,N,n}(p)(h(x)) \bigg|_{x=c_i} = 0, \quad 1 \leq m \leq M_i.$$ 

Therefore the only contribution in the expression for $p^{(j)}(c_i)$ when $1 \leq j \leq M_i$ is when $k = j$, giving

$$p^{(j)}(c_i) = \sum_{n=j}^{N-1} \frac{n!}{(n-j)!} c_i^{n-j} R_{h,N,n}(p)(0), \quad 1 \leq j \leq M_i.$$
For \( p \equiv (R_{h,N,0}(p), \ldots, R_{h,N,N-1}(p)) \) and \( q \equiv (R_{h,N,0}(q), \ldots, R_{h,N,N-1}(q)) \) the inner product (3.2) can thus be written as

\[
\langle p, q \rangle = \int \left( R_{h,N,0}(p)(h(x)) \ldots R_{h,N,N-1}(p)(h(x)) \right) dM(x) \begin{pmatrix}
R_{h,N,0}(q)(h(x)) \\
R_{h,N,1}(q)(h(x)) \\
\vdots \\
R_{h,N,N-1}(q)(h(x))
\end{pmatrix},
\]

\[
+ \left( R_{h,N,0}(p)(0) \ldots R_{h,N,N-1}(p)(0) \right) L \begin{pmatrix}
R_{h,N,0}(q)(0) \\
R_{h,N,1}(q)(0) \\
\vdots \\
R_{h,N,N-1}(q)(0)
\end{pmatrix},
\]

where \( M \) is the \( N \times N \) matrix of measures

\[
dM(x) = \begin{pmatrix}
d\mu(x) & x \, d\mu(x) & \cdots & x^{N-1} \, d\mu(x) \\
x \, d\mu(x) & x^2 \, d\mu(x) & \cdots & x^N \, d\mu(x) \\
x^2 \, d\mu(x) & x^3 \, d\mu(x) & \cdots & x^{N+1} \, d\mu(x) \\
\vdots & \vdots & \ddots & \vdots \\
x^{N-1} \, d\mu(x) & x^N \, d\mu(x) & \cdots & x^{2N-2} \, d\mu(x)
\end{pmatrix}
\]

and \( L \) is the matrix

\[
L(i, j) = \sum_{i=1}^{M} \sum_{j=1}^{M_i} \lambda_{i,j} L(i, j)
\]

with \( L(i, j) \) the \( N \times N \) matrix

\[
L(i, j) = \begin{pmatrix}
0 \\
\vdots \\
0 \\
j! \\
\vdots \\
\frac{k!}{(k-j)!} c_i^{k-j} \\
\vdots \\
\frac{(N-1)!}{(N-1-j)!} c_i^{N-1-j}
\end{pmatrix}
\]

with entries

\[
L_{k,n}(i, j) = \frac{k! \, n!}{(k-j)! \, (n-j)!} c_i^{n+k-2j}, \quad j \leq k, n \leq N - 1.
\]

It is clear that \( L(i, j) \) is positive definite, hence \( L \) is also positive definite when all \( \lambda_{i,j} \geq 0 \). If \( p_n(x) \) \((n = 0, 1, 2, \ldots)\) are the orthonormal polynomials with respect to the Sobolev inner product (3.2), then we can write the polynomials \( p_{kN+l}(x) \) \(0 \leq l < N\) using the basis functions (3.3):

\[
p_{kN+l}(x) = \sum_{n=0}^{N-1} x^n R_{h,N,n}(p_{kN+l})(h(x)), \quad l = 0, 1, \ldots, N - 1.
\]
The matrix polynomials

\[ P_n(x) = \begin{pmatrix} R_{h,N,0}(p_{nN})(x) & \cdots & R_{h,N,N-1}(p_{nN})(x) \\ R_{h,N,0}(p_{nN+1})(x) & \cdots & R_{h,N,N-1}(p_{nN+1})(x) \\ \vdots & \ddots & \vdots \\ R_{h,N,0}(p_{nN+N-1})(x) & \cdots & R_{h,N,N-1}(p_{nN+N-1})(x) \end{pmatrix}, \]

are then orthonormal with respect to the matrix of measures \( M(h^{-1}) \) to which a mass point at 0 is added, with weight given by the matrix \( L \). The matrix of measures \( M(h^{-1}) \) is given by

\[ \int F(x) \, dM(h^{-1}(x)) = \int F(h(x)) \, dM(x), \]

where \( F : \mathbb{R} \to \mathbb{R}^N \) is a vector function such that \( F(h) \in L_1(M) \). In this way Sobolev orthogonal polynomials (with a discrete Sobolev part) can always be expressed as orthogonal matrix polynomials, where the spectral matrix of measures has a mass point at the origin. Note that the matrix polynomial \( P_k(x) \) is of degree \( k \) with a leading coefficient which is a lower triangular matrix because the degree of \( R_{h,N,n}(p_{kN+l}) \) is less than \( k \) whenever \( n > l \).

3.2 Perturbation of a measure on the real line by finitely many function values.

As a second example we consider the inner product

\[ \langle f, g \rangle = \int f(x)g(x) \, d\mu(x) + \left( \sum_{k=0}^{N-1} a_k f(c_k) \right) \left( \sum_{k=0}^{N-1} a_k g(c_k) \right), \]

where \( f, g \) are real functions, \( \mu \) is a positive measure on the real line and \( a_k, c_k \in \mathbb{R} \) \((k = 0, \ldots, N - 1)\). When \( N = 1 \) then this is just an inner product in \( L_2 \) with respect to the measure \( \mu \) to which a mass \( a_0^2 \) is added at the point \( c_0 \). The case \( N = 2 \) with \( a_0 = -a_1 \) is basically an inner product involving differences, as introduced recently by Bavinck [2] [3].

If we consider the polynomial

\[ h(x) = \prod_{k=0}^{N-1} (x - c_k), \]

then \( h \) vanishes at the points \( c_k \) where the function values are evaluated in the inner product, and hence

\[ \langle f, hg \rangle = \int h(x)f(x)g(x) \, d\mu(x) = \langle hf, g \rangle, \]

which immediately implies that the orthonormal polynomials \( (p_n)_n \) for this inner product satisfy a \((2N+1)\)-term recurrence formula of the form (1.3). Expanding a polynomial \( p \) in the basis (3.3) gives

\[ p(x) = \sum_{n=0}^{N-1} x^n R_{h,N,n}(p(h(x))). \]
Observe that
\[ p(c_k) = \sum_{n=0}^{N-1} c_n^p R_{h,N,n}(p)(0), \]
hence for \( p \equiv (R_{h,N,0}(p), \ldots, R_{h,N,N-1}(p)) \) and \( q \equiv (R_{h,N,0}(q), \ldots, R_{h,N,N-1}(q)) \) we have
\[
\left( \sum_{k=0}^{N-1} a_k f(c_k) \right) \left( \sum_{k=0}^{N-1} a_k g(c_k) \right) = (R_{h,N,0}(p)(0) \ldots R_{h,N,N-1}(p)(0)) L \begin{pmatrix} R_{h,N,0}(q)(0) \\ R_{h,N,1}(q)(0) \\ \vdots \\ R_{h,N,N-1}(q)(0) \end{pmatrix},
\]
where
\[
L = \begin{pmatrix} \sum_{k=0}^{N-1} a_k \\ \sum_{k=0}^{N-1} a_k c_k \\ \vdots \\ \sum_{k=0}^{N-1} a_k c_k^{N-1} \end{pmatrix} \begin{pmatrix} \sum_{k=0}^{N-1} a_k \\ \sum_{k=0}^{N-1} a_k c_k \\ \vdots \\ \sum_{k=0}^{N-1} a_k c_k^{N-1} \end{pmatrix}.
\]
The inner product (3.5) in the linear space of scalar polynomials thus corresponds to an inner product in \( \mathbb{L}^2 \) for the measure \( \mathbf{M}(h^{-1}) \), with \( \mathbf{M} \) given by (3.4), to which a Dirac measure at 0 is added with weight given by the positive definite matrix \( L \). Moreover, the matrix polynomials
\[
P_n(x) = \begin{pmatrix} R_{h,N,0}(p_nN)(x) & \ldots & R_{h,N,N-1}(p_nN)(x) \\ R_{h,N,0}(p_nN+1)(x) & \ldots & R_{h,N,N-1}(p_nN+1)(x) \\ \vdots & \ddots & \vdots \\ R_{h,N,0}(p_nN+N-1)(x) & \ldots & R_{h,N,N-1}(p_nN+N-1)(x) \end{pmatrix}
\]
are orthonormal with respect to \( \mathbf{M}(h^{-1}) + L \delta_0 \).

The special case when one adds to the \( L_2(\mu) \) inner product a part dealing with the \((N-1)\)st difference, i.e.,
\[
\sum_{k=0}^{N-1} a_k f(c_k) = \Delta^{N-1} f(c),
\]
corresponds to the choice \( c_k = c + k \delta \) and \( a_k = (-1)^k \binom{N-1}{k} \). Observe that in this case
\[
L = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ (-\delta)^{N-1}(N-1)! \end{pmatrix}
\]
so that \( L \) contains zeros everywhere, except for the entry in the lower right corner. This case covers the inner products considered by Bavinck [2] [3]. The limiting case where \( \delta \to 0 \) corresponds to a discrete Sobolev inner product with a \((N-1)\)st derivative at the point \( c \). The general discrete Sobolev inner product (3.2) can also be obtained as a limiting case of (3.5) by letting some of the \( c_k \) coincide and taking appropriate coefficients.
4. Krein’s theorem revisited

Suppose that the spectrum $\sigma(J)$ of a (tridiagonal) Jacobi matrix $J$ is denumerable. If the set of accumulation points of the spectrum $\sigma(J)$ is finite, then a complete characterization of the derived set $\sigma(J)'$ is given by M.G. Krein [14] [6, Chapter IV, Section 6]:

**Krein’s theorem.** Suppose $J$ is a bounded Jacobi matrix. Then every accumulation point of $\sigma(J)$ is a zero of the polynomial $h(x)$ of degree $N$ if and only if the operator $h(J)$ is compact.

The relationship between polynomials satisfying a higher order recurrence relation an orthogonal matrix polynomials enables us to give a short proof of this result.

**Proof of Krein’s theorem.** The infinite matrix $h(J)$ is a banded matrix with bandwidth $2N + 1$, and can thus be written as

$$h(J) = D + \sum_{j=1}^{N} (V^*)^j A_j + \sum_{j=1}^{N} B_j V^j,$$

where $D, A_1, B_1, \ldots, A_N, B_N$ are diagonal matrices and $V$ is the shift operator that acts as $(V\psi)_n = \psi_{n+1}$. A diagonal matrix is compact if and only if its entries tend to zero, and compact operators on a Hilbert space form a two-sided ideal in the set of bounded operators on this Hilbert space. Hence the boundedness of the shift operator implies that $h(J)$ is compact if and only if the entries of $h(J)$ tend to zero along the diagonals. If we write $h(J)$ as a block Jacobi matrix

$$h(J) = \begin{pmatrix} E_0 & D_1 & \cdots & & \cdots \\ D_1^* & E_1 & D_2 & \cdots & \cdots \\ & D_2^* & E_2 & \cdots & \cdots \\ & & \ddots & \ddots & \ddots \\ & & & & \end{pmatrix},$$

where $E_k, D_k$ are $N \times N$ matrices and $D_k$ are lower triangular, then the compactness of $h(J)$ implies that $E_k$ and $D_k$ converge towards the zero matrix. A compact operator has a denumerable spectrum with zero as the only accumulation point. If $\mu$ is the spectral measure for $J$ (with corresponding orthogonal polynomials $p_n(x)$), then $M(h^{-1})$ is the matrix of measures for which the matrix polynomials $P_n(x)$ corresponding with $h(J)$ are orthogonal, where

$$dM(x) = \begin{pmatrix} d\mu(x) & x d\mu(x) & \cdots & x^{N-1} d\mu(x) \\ x d\mu(x) & x^2 d\mu(x) & \cdots & x^N d\mu(x) \\ x^2 d\mu(x) & x^3 d\mu(x) & \cdots & x^{N+1} d\mu(x) \\ \vdots & \vdots & \ddots & \vdots \\ x^{N-1} d\mu(x) & x^N d\mu(x) & \cdots & x^{2N-2} d\mu(x) \end{pmatrix}.$$

If $\sigma(h(J))$ is the spectrum of $h(J)$, then it follows that the spectrum of $J$ is given by $h^{-1}(\sigma(h(J)))$. We know that $\sigma(h(J))$ has only one accumulation point at zero, which therefore corresponds to accumulation points of $J$ at $h^{-1}(0)$, which are the zeros of the polynomial $h(x)$.

Conversely, if we know that $\sigma(J)$ is denumerable with accumulation points at the zeros of $h$, then the spectrum of $h(J)$ is given by $h(\sigma(J))$ and is therefore also denumerable with accumulation points at $h(h^{-1}(0)) = 0$, which makes $h(J)$ a compact operator. □
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