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ON ORTHOGONAL MATRIX POLYNOMIALS

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In this paper we deal with orthogonal matrix polynomials. First of all, we establish some basic notations and results we need later.

A matrix polynomial P is a matrix whose entries are polynomials, or, equivalently, a combination $P(t) = A_0 + A_1 t + \cdots + A_n t^n$, where $A_0, \cdots, A_n$ are numerical matrices (the size of all the matrices which appear in this paper is $N \times N$).

A positive definite matrix of measures W is a matrix whose entries are Borel measures and such that for any Borel set $A \in \mathbb{R}$, the numerical matrix $W(A)$ is positive semidefinite.

A sequence of matrix polynomials $(P_n)_n$, $\operatorname{dgr}(P_n) = n$, is orthonormal with respect to a positive definite matrix of measures W if:

$$\int P_n(t) dW(t) P_m^*(t) = \delta_{n,m} Id.$$

Matrix orthonormality is equivalent to the following three-term matrix recurrence relation

$$tP_n(t) = A_{n+1}P_{n+1}(t) + B_n P_n(t) + A_n^* P_{n-1}(t),$$

with initial condition $P_{-1} = \theta$ and P_0 a nonsingular numerical matrix, and where the B_n's are hermitian and the A_n's are nonsingular (see [1, 4, 8]). Using the polar decomposition of a matrix, the A_n's can be taken to be positive definite, while the QR decomposition of Francis and Kublanovskaja allows us to take the A_n's to be lower triangular matrices.

We can associate to the sequence of orthogonal matrix polynomials $(P_n)_n$ the $(2N+1)$-banded infinite Hermitian matrix which is called the N-Jacobi matrix

$$J = \begin{pmatrix} B_0 & A_1 & & & \\ A_1^* & B_1 & A_2 & & \\ & A_2^* & B_2 & A_3 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}.$$

As in the scalar case, the polynomials of the second kind are defined as

$$Q_n(z) = \int \frac{P_n(z) - P_n(t)}{z - t} dW(t).$$

The sequence $(Q_n)_n$ satisfies the same three-term recurrence relation as that satisfied by $(P_n)_n$ but with initial conditions $Q_0 = \theta$, Q_1 a nonsingular numerical matrix.

The paper is divided in two parts. In the first one we show a close link between scalar polynomials satisfying higher order recurrence relations and orthogonal matrix polynomials. Using this relationship, we give a nontrivial interpretation of scalar orthogonality as matrix orthogonality, and, as a consequence, we will see that orthogonal matrix polynomials are going to be a useful tool to study some problems in the classical theory of orthogonal polynomials with respect to a positive measure. In the second part, we will give a survey of some recent results on orthogonal matrix polynomials in the real line: properties of their zeros, quadrature formulae, asymptotic behaviour, density results, etc.

2 SCALAR POLYNOMIALS AND MATRIX POLYNOMIALS

According to this plan, the starting point for the first part will be the well-known Favard's theorem which establishes that for a sequence of polynomials $(p_n)_n$ ($\mathrm{dgr}(p_n) = n$) the following conditions are equivalent:

- $(p_n)_n$ is a sequence of orthonormal polynomials with respect to a positive measure.
- There are two sequences $(a_n)_n$ ($a_n \neq 0$, $n \in \mathbb{N}$), $(b_n)_n$ for which

$$tp_n(t) = a_{n+1}p_{n+1}(t) + b_n p_n(t) + a_n p_{n-1}(t). \tag{1}$$

The formula (1) is known as the three-term recurrence relation.

In the late 80's the following problem, which can be considered as an extension for higher order recurrence relation of Favard's theorem, arises: *To describe the canonical orthogonality for a sequence of polynomials $(p_n)_n$, ($\mathrm{dgr}(p_n) = n$) which satisfies*

$$t^N p_n(t) = c_{n,0}p_n(t) + \sum_{k=1}^{N} \left(\bar{c}_{n,k}p_{n-k}(t) + c_{n+k,k}p_{n+k}(t)\right), \tag{2}$$

where $c_{n,0}$ is real, $c_{n,N} \neq 0$, $n \in \mathbb{N}$, and $p_k = 0$ for $k < 0$.

Sequences of polynomials satisfying the previous $(2N+1)$-term recurrence formula appear in the context of the so-called discrete Sobolev inner products, i.e., inner products obtained by perturbing with a discrete differential part the inner product defined by a positive measure:

$$< p, q >= \int_{\mathbb{R}} p(t)q(t)d\mu(t) + \sum_{k,m=1}^{n} M_{k,m}p^{(k)}(x_k)q^{(m)}(x_m),$$

where μ is a positive measure, $M_{k,m} \geq 0$ and x_k, x_m are real.

The solution of this problem is certainly unexpected, and roughly speaking can be established as follows: If $(p_n)_n$ satisfy (2) then the polynomials $p_n(t)$ can be splitted up, attending to the congruence of the exponents of t modulus N, to get a sequence of matrix polynomials $(P_n)_n$ which is orthonormal in the real line with respect to a positive definite matrix of measures. And conversely, given a sequence $(P_n)_n$ of orthogonal matrix polynomials with respect to a positive definite matrix of measures, a sequence of scalar polynomials, satisfying the recurrence (2), can be rebuilt from the polynomials in the rows of each P_n.

Besides the relationship this solution is showing, the result has an important consequence which we will explain later, but which it is worthy to point out here: this result provides a non-trivial interpretation of scalar orthogonality (i.e. orthogonality with respect to a positive measure) as matrix orthogonality. This non-trivial interpretation will be the key to apply the matrix orthogonality to solve some problems in the theory of orthogonal polynomials with respect to a positive measure.

To establish the solution of the previous problem in full, we need to introduce the following operators which will be used to split up the scalar polynomials: for a natural number N, the operators $R_{N,m}$, $m = 0, 1, \cdots, N-1$ are defined in the linear space of polynomials $\mathbb{P}$ as

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

that is, the operator $R_{N,m}$ takes from the polynomial p those powers of t congruent with m modulus N, then removes the common factor t^m and changes t^N to t.

We can now establish the following theorem which is an extension of Favard's theorem for higher order recurrence relation:

Theorem 1. *([4])*
If the polynomials $(p_n)_n$ (dgr $(p_n) = n$) satisfy a $(2N+1)$-term recurrence formula then there exists a positive definite matrix of measures $\mu = (\mu_{m,m'})_{m,m'=0,\cdots,N-1}$ such that the polynomials $(p_n)_n$ are orthonormal with respect to the inner product

$$B(p,q) = \sum_{0\le m,m'\le N-1} \int_R R_{N,m}(p) R_{N,m'}(q) d\mu_{m,m'}.$$

Using this theorem the relationship between scalar polynomials satisfying a higher order recurrence relation and matrix orthogonal polynomials follows:

Theorem 2. *([11])*
Let $p_n(t)$ $(n = 0,1,2,\cdots)$ $(dgr(p_n) = n)$ be scalar polynomials satisfying a $(2N+1)$-term recurrence relation and let $(P_n)_n$ be matrix polynomials given by

$$P_n(t) = \begin{pmatrix} R_{N,0}(p_{nN})(t) & \dots & R_{N,N-1}(p_{nN})(t) \\ R_{N,0}(p_{nN+1})(t) & \dots & R_{N,N-1}(p_{nN+1})(t) \\ \vdots & \ddots & \vdots \\ R_{N,0}(p_{nN+N-1})(t) & \dots & R_{N,N-1}(p_{nN+N-1})(t) \end{pmatrix}.$$

Then this sequence of matrix polynomials is orthonormal in the real line with respect to a positive definite matrix of measures.
Conversely, if $P_n = (P_{n,m,j})_{m,j=0}^{N-1}$ is a sequence of orthonormal matrix polynomials, then the scalar polynomials defined by

$$p_{nN+m}(t) = \sum_{j=0}^{N-1} t^j P_{n,m,j}(t^N), \qquad (n \in \mathbb{N}, 0 \le m \le N-1),$$

satisfy a $(2N+1)$-term recurrence formula.

We are now ready to show how to use Theorem 1 to give a non-trivial interpretation of scalar orthogonality as matrix orthogonality. For the sake of simplicity, we take $N = 2$. So, let $(p_n)_n$ be scalar polynomials which are orthonormal with respect to a positive measure, or equivalently:

$$tp_n(t) = a_{n+1}p_{n+1}(t) + b_np_n(t) + a_np_{n-1}(t). \tag{3}$$

Iterating (3) we get a five-term recurrence relation

$$t^2p_n(t) = \alpha_{n+2}p_{n+2}(t) + \beta_{n+1}p_{n+1}(t) + \gamma_np_n(t) + \beta_np_{n-1}(t) + \alpha_np_{n-2}(t).$$

So, there exists a 2×2 positive definite matrix of measures

$$W = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix}$$

such that the polynomials $(p_n)_n$ are orthonormal with respect to W in the sense of Theorem 1, that is,

$$\sum_{i,j=0}^{1} \int_{\mathbb{R}} R_{2,i}(p_n)R_{2,j}(p_m)dw_{i,j} = \delta_{n,m}.$$

A natural question arises: is there some relationship between the measure μ with respect to which the polynomials $(p_n)_n$ are orthonormal and the positive definite matrix of measures W?

First of all, it is not difficult to see that each positive measure μ for which

$$\int p_n p_m d\mu = \delta_{n,m}$$

gives a positive definite matrix of measures W_μ with respect to which $(p_n)_n$ are also orthonormal; this matrix of measures is defined as follows:

$$W_\mu = \begin{pmatrix} \psi(\mu) & \psi(t\mu) \\ \psi(t\mu) & \psi(t^2\mu) \end{pmatrix},$$

where $\psi(\mu)$ is the image measure of μ under $\psi(t) = t^2$. Indeed, the inner product defined by W_μ in the space of polynomials is just the same as that defined by μ.

But, the key of the question is that other positive definite matrices of measures W can exist which are not of the form W_μ. These matrices of measures may give (and in fact they do give) new information about the polynomials $(p_n)_n$.

We illustrate this with two examples.

The first one is related to the asymptotic properties of the derivatives of a sequence $(p_n)_n$ of scalar polynomials orthonormal with respect to a positive measure. Indeed, it is very well-known the formula:

$$\frac{1}{\sum_n |p_n(x)|^2} = \sup\{\mu(\{x\}) : \mu \text{ is a weight for } (p_n)_n \}.$$

However, similar formulas for the derivatives of the polynomials did not seem to be known: to get them it is necessary to consider the matrix orthogonality for the scalar polynomials $(p_n)_n$ as explain before; then, the following formula, where the matrix weights for $(p_n)_n$ appear in an essential way, can be proved

$$\frac{1}{\sum_n |p_n'(0)|^2} = \sup\{w_{22}(\{0\}) - \frac{|w_{12}|^2(\{0\})}{w_{1,1}(\{0\})} : W = (w_{i,j})_{i,j=1}^2$$
$$W \text{ matrix weight for } (p_n)_n \}.$$

Other formulas for higher derivatives evaluated at any real number can be found in [4].

The second example can be found in [11], and it consists in using the matrix interpretation of scalar orthogonality to get a new and very simple proof of Krein's theorem regarding orthogonal polynomials with a spectrum with finitely many accumulation points.

These applications of matrix orthogonality to solve some problems of scalar orthogonality give a new and strong motivation to do a systematic study of matrix orthogonality in the real line. The first steps towards this systematic study can be found in [5], [6], [7], [8], [9] and [10], although some sparse results have been obtained during the last fifty years; for instance, Krein proved some results for matrix moment problem (using operator theory) ([19], [20]); more recently, in the 80's, matrix orthogonality in the real line has appeared in connection with scattering and prediction theories ([14], [17]), and the analogous to Favard's theorem has been established ([2]); other related results can be found in [1], [12], [13], [18], [21], [22] or [23].

3 SOME RESULTS ON ORTHOGONAL MATRIX POLYNOMIALS

The second part of this paper will be devoted to show some recent results on orthogonal matrix polynomials which can be considered as the starting point for the systematic study we mentioned above.

The first results we are going to consider are related to the properties of zeros.

As usual, we say that a is a zero of the matrix polynomial $P(t)$ if a is a zero of $\det(P(t))$, i.e., if $P(a)$ is a singular matrix or, equivalently, 0 is an eigenvalue of $P(a)$.

Given a sequence of orthogonal matrix polynomials $(P_n)_n$, we have the following properties for the zeros of the polynomial P_n:

- They can have multiplicity bigger than one but always bounded by N, (let us remind that N is the size of the matrices we are considering).
- The zeros are real.
- There also exists a separation property between the zeros of P_n and the zeros of P_{n+1} but weaker than in the scalar case.

These properties can be easily deduced from the important fact that the zeros of P_n are just the eigenvalues of the truncated N-Jacobi matrix of size nN (of course, with the same multiplicity) associated to the polynomials $(P_n)_n$ (see [8]).

Although these properties are quite natural, they are not complete in the following sense: in the scalar case, a is a zero of $p(t)$ if $p(a)=0$, but in the matrix case, a is a zero of $P(t)$ does not imply $P(a)=\theta$, a is a zero of $P(t)$ is equivalent to say that 0 is an eigenvalue of $P(a)$, but then, something must be said about the eigenvectors of $P(a)$ associated to 0. The following property, which we have called *the fundamental property of the zeros* (the reasons for this name will appear clear when we have shown the important consequences of this property), gives an answer to this question (see [5]):

> If a is a zero of P_n of multiplicity p, then the rank of $P_n(a)$ is just $N-p$ and the matrices $\left(\operatorname{Adj}\left(P_n(t)\right)\right)^{(p-1)}(a)$ and $P^*_{n-1}(a)A_n$ define two isomorphisms between the space of right eigenvectors and the space of left eigenvectors of $P_n(a)$ associated to 0. The inverse of $P^*_{n-1}(a)A_n$ is given by the matrix $Q_n(a)$ (A_n is the matrix which appears in the three-term recurrence relation for $(P_n)_n$, and Q_n is the n-th polynomial of the second kind).

This property for the zeros of orthogonal matrix polynomials is analogous to the fact that they are real and simple in the scalar case. Indeed, since in the scalar case the zeros are real and simple, one can expand the ratio $\dfrac{p(z)}{p_n(z)}$ (where p is a polynomial of degree at most n) into simple fractions:

$$\frac{p(z)}{p_n(z)}=\sum_{i=1}^{n}\frac{b_i}{z-a_i};$$

as a consequence, we can write $\dfrac{p(z)}{p_n(z)}$ as the Hilbert transform of the discrete measure $\mu_n=\displaystyle\sum_{i=1}^{n}b_i\delta_{a_i}$; we can now deduce properties of the measure μ_n from the ratio $\dfrac{p(z)}{p_n(z)}$, and viceversa. In the matrix case, since the zeros can have multiplicity bigger than one, one does not expect to be able to expand the ratio $P_n^{-1}(z)P(z)$ (or $P(z)P_n^{-1}(z)$) in simple fractions (and then to be able to write this ratio as the Hilbert transform of a matrix of discrete measures) as in the scalar case. However, from the fundamental property it follows that although the multiplicity of the zeros of P_n can be bigger than one the decomposition

$$P(z)P_n^{-1}(z)=\sum_{k=1}^{m}\frac{C_k}{z-x_k},\quad \operatorname{dgr}\,(P)\le n-1$$

is always possible.

The fundamental property is also the key to establish the following quadrature formulae, where an explicit expression for the weights is given (see [5]; for other quadrature formulas lacking an explicit expression for the weights see [8], [22])

Quadrature formulae for orthogonal matrix polynomials. *Let $(P_n)_n$ be a sequence of orthonormal polynomials with respect to the positive definite matrix of measures W, and let $x_{n,k}$, $k = 1, \cdots, m$, be the different zeros of P_n ordered in increasing size and taking into account their multiplicities and let*

$$\Gamma_{n,k} = \frac{1}{(det(P_n(t))^{(l_k)}(x_{n,k})} \left(Adj(P_n(t))\right)^{(l_k-1)}(x_{n,k})Q_n(x_{n,k}),$$

where l_k is the multiplicity of $x_{n,k}$. Then

(a) *If the degree of P is less than $2n-1$ then*

$$\int P(t)d\mu(t) = \sum_{k=1}^{m} P(x_{n,k})\Gamma_{n,k}.$$

(b) *$\Gamma_{n,k}$ are positive semidefinite matrices of rank l_k, $k = 1, \cdots, m$.*

We can now use this quadrature formulae to extend to the matrix case one of the main asymptotic result in the scalar case: the Markov's theorem (see [5]).

Markov's theorem for orthogonal matrix polynomials. *Let $(P_n)_n$ orthogonal matrix polynomials with respect to a positive definite and determinate matrix of measures W (as in the scalar case, determinate means that no other matrix of measures has the same moments as those of W), then*

$$\lim_n P_n^{-1}(z)Q_n(z) = \int \frac{dW(t)}{z-t} \quad \text{for } z \in \mathbb{C} \setminus \Gamma,$$

where Γ is certain set of real numbers containing the support of W, and the convergence is uniform in compact sets.

We remark that in the matrix version of Markov's theorem, the matrices P_n^{-1} and Q_n must be multiplied in the order $P_n^{-1}Q_n$, otherwise the result could be false.

The quadrature formula can also be used to obtain some ratio asymptotic results for orthogonal matrix polynomials (see [6]).

Ratio asymptotics for orthogonal matrix polynomials. *Let $(P_n)_n$ be orthonormal matrix polynomials with respect to the positive definite matrix of measures W, satisfying*

$$\lim_n A_n = A, \quad \lim_n B_n = B,$$

then

$$\lim_n P_{n-1}(z)P_n^{-1}(z) = \left(\int \frac{dW_{A,B}}{z-t}\right) A \quad z \in \mathbb{C} \setminus \Gamma,$$

where Γ is certain bounded set of real numbers containing the support of W and the convergence is uniform in compact sets. $W_{A,B}$ is the matrix of measures with respect to which the matrix polynomials $(R_n)_n$ satisfying the three-term recurrence relation

$$tR_n(t) = AR_{n+1}(t) + BR_n(t) + AR_{n-1}(t)$$

are orthonormal.

As for the matrix version of Markov's theorem, the matrix polynomials P_n^{-1} and P_{n-1} must be multiplied in the order $P_{n-1}P_n^{-1}$, otherwise the result could be false.

A partial extension of Blumenthal theorem has been also proved for this matrix Nevai class, i.e., the class of orthogonal matrix polynomials for which

$$\lim_n A_n = A, \quad \lim_n B_n = B.$$

In this case, we assume the stronger condition that the diagonals of the N-Jacobi matrix associated to the polynomials $(P_n)_n$ are convergent sequences (actually, these sequences are the same as in the $(2N+1)$-term recurrence relation associated to the polynomials $(P_n)_n$ in the sense explained in the first part of this paper). We write c_k for the limit of the k-th updiagonal, $k = 0, 1, \cdots, N$ (since the N-Jacobi matrix is a $(2N+1)$-banded hermitian matrix these N updiagonals have all the information). Then, the support of the orthogonalizing matrix of measures for $(P_n)_n$ is a compact interval plus, possibly, two sequences of real numbers outside this interval which tend to its endpoints. This interval is given by

$$[c_0 + \inf_{x\in[-\pi,\pi]} t(x), c_0 + \sup_{x\in[-\pi,\pi]} t(x)],$$

where $t(x)$ is the trigonometric polynomial

$$t(x) = \left(\sum_{k=1}^{N} 2\Re(c_k)T_k(\cos x)\right) - \left(\sum_{k=1}^{N} 2\Im(c_k)\sin x U_{k-1}(\cos(x))\right) = 2\Re\left(\sum_{k=1}^{N} c_k e^{ikx}\right),$$

and $(T_k)_k, (U_k)_k$ are the Chebyshev polynomials of the first and second kind, respectively (see [8]).

The property (b) of the weights in the quadrature formulae is the key to solve the following density problem for the truncated moment problem: let $(P_n)_n$ be a sequence of orthogonal matrix polynomials with respect to the positive definite matrix of measures W; we write

$$V_n = \{\nu : \nu \text{ is a positive definite matrix of measures for which}$$
$$\int t^k d\nu(t) = \int t^k dW(t), k = 0, \cdots, n\}.$$

then

Theorem. *([9]) If $\nu \in V_{2n-2}$ the following conditions are equivalent*

(1) *ν is an extremal point, in the sense of convexity, of V_{n-1}.*
(2) *The space of matrix polynomials of degree less than n is dense in $L^2(\nu)$.*
(3) *There exists a matrix A, with $A_n A = A^* A_n^*$, such that*

$$\nu = \sum_{i=1}^{m} G_i \delta_{x_i},$$

where x_i are the different zeros of $P_n(t) - AP_{n-1}(t)$ and G_i are the matrices which appear in the partial fraction decomposition

$$(P_n(z) - AP_{n-1}(z))^{-1}(Q_n(z) - AQ_{n-1}(z)) = \sum_{i=1}^{m} \frac{G_i}{z - x_i}.$$

This theorem have important divergences with its scalar version. Indeed, in the scalar case, the points of the support of the extremal measures support the maximum mass in V_{2n-2} which at the point x is

$$\frac{1}{\sum_{k=0}^{n-1} p_k^2(x)}.$$

This property is no longer true for the matrix case: the matrices in V_{2n-2} extremal in V_{n-1} may not support the maximum mass in V_{2n-2}. This happens exactly when the mass is a nonsingular matrix. In such a case the polynomial $P_n(z) - AP_{n-1}(z)$ has a zero of multiplicity N (the biggest possible) at the point x; in that case A is given by $A = P_n(x)P_{n-1}^{-1}(x)$ (see [9]).

The following result is also related to density questions, in this case for the space $L^1(W)$, W a positive definite matrix of measures (see [10] for the definition of the L^p spaces for a positive definite matrix of measures). The result is a partial extension to the matrix case of the well-known Naimark's theorem which characterizes those measures among the convex set of measures having the same moments such that the linear space of polynomials is dense in L^1: just the extremal measures (in the sense of convexity).

Theorem. *([10]) Let W be a definite positive matrix of measures with finite moments, then*

(1) *The set*

$$V_n = \{\nu : \nu \text{ is a positive definite matrix of measures for which } \int t^k d\nu(t) = \int t^k dW(t), k \in \mathbb{N}\}$$

is a compact and convex set.

(2) *For $\nu \in V$, let $M(t)$ be the matrix of Radon-Nikodym derivatives of the elements of ν with respect to the trace measure. Let*

$$0 \leq \lambda_1(t) \leq \cdots \leq \lambda_N(t)$$

be the eigenvalues of $M(t)$. If there exists a constant $c > 0$, such that $\lambda_1(t) \geq c$ then the space of matrix polynomials is dense in $L^1(\nu)$ if and only if ν is an extremal point, in the convexity sense, of V.

The existence of extremal points in the convex set V follows from the compactness of V.

The hypothesis in (2) is superfluous for the scalar case: in that case the trace of W coincides with W and then the matrix of the Radon-Nikodym derivatives is $M(t) = 1$, hence the eigenvalues of $M(t)$ are reduced in this case to 1. In the matrix case, the eigenvalues of $M(t)$ have a more complicated structure, and to extend Naimark's theorem to the matrix case we need, as an additional hypothesis, that the eigenvalues of $M(t)$ do not approach to 0.

Some general results concerning orthogonal matrix polynomials and differential equations have recently been obtained (see [15, 16] for some examples of orthogonal matrix polynomials satisfying differential equations). In [7] the following problem has been studied: consider the second order differential operators:

$$l_{2,L} = A_2 D'' + A_1 D' + A_0 D^0,$$

and

$$l_{2,R} = D'' A_2 + D' A_1 + D^0 A_0,$$

where A_2, A_1, A_0 are certain matrix functions. The problem is: for which matrices of measures W the operator l_2 is symmetric with respect to the inner product defined by W?

The noncommutativity of the matrix product introduces a strong difference between the left and right hand side. Indeed, for $l_{2,R}$ the problem is equivalent to the fact that the orthonormal matrix polynomials $(P_n)_n$ with respect to W satisfy the differential equation

$$l_{2,R}(P_n) = \Gamma_n P_n,$$

for certain hermitian matrices Γ_n. But this is not the case for $l_{2,L}$.

However, there is a classification result for the left hand side case:

Theorem. *([7]) The matrices of measures whose matrix inner product has a symmetric left hand side second order differential operator are of the form D^*XD, where D is a nonsingular numerical matrix and $X = \nu I$, where ν is a classic measure, that is, the Jacobi, Laguerre or Hermite weights up to a linear change of variable.*

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