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Orthogonal matrix polynomials, scalar-type Rodrigues' formulas and Pearson equations ☆

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Abstract

Some families of orthogonal matrix polynomials satisfying second-order differential equations with coefficients independent of n have recently been introduced (see [Internat. Math. Res. Notices 10 (2004) 461–484]). An important difference with the scalar classical families of Jacobi, Laguerre and Hermite, is that these matrix families do not satisfy scalar type Rodrigues' formulas of the type $(\Phi^n W)^{(n)} W^{-1}$, where Φ is a matrix polynomial of degree not bigger than 2. An example of a modified Rodrigues' formula, well suited to the matrix case, appears in [Internat. Math. Res. Notices 10 (2004) 482].

In this note, we discuss some of the reasons why a second order differential equation with coefficients independent of n does not imply, in the matrix case, a scalar type Rodrigues' formula and show that scalar type Rodrigues' formulas are most likely not going to play in the matrix valued case the important role they played in the scalar valued case. We also mention the roles of a scalar-type Pearson equation as well as that of a noncommutative version of it.

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1. Introduction

This introduction is organized in three parts: part 1 gives a description of the problem and a formulation of our point of view; part 2 describes some of the previous results that are pertinent here and how they motivate some of the issues taken up in later sections. Part 2 should give the reader a general idea of the contents of this paper and finally part 3 gives a rather precise guide to the results in this paper.

We start by recalling the basic setup.

Definition 1.1. We say that an $N \times N$ matrix of measures supported on the real line is a (positive definite) weight matrix if

- (1) W(A) is positive semidefinite for any Borel set $A \subset \mathbb{R}$;
- (2) W has finite moments of every order, and
- (3) $\int P(t) dW(t) P^*(t)$ is nonsingular whenever the leading coefficient of the matrix polynomial P is nonsingular.

Condition (3) is necessary and sufficient to guarantee the existence of a sequence $(P_n)_n$ of matrix polynomials orthogonal with respect to W, P_n of degree n and with nonsingular leading coefficient. Throughout this paper, we always consider weight matrices W having a smooth absolutely continuous derivative W' with respect to Lebesgue measure; assuming that this matrix derivative W' is positive definite at infinitely many real numbers, condition (3) above holds automatically. For other basic definitions and results on matrix orthogonality, see for instance [Be,D2,D1,DP,Ge,K1,K2].

Among all possible families of orthogonal polynomials, either in the scalar or the matrix valued case, it is natural to concentrate on those that posses *some extra property*. It is clear that these families are likely to play, by their own nature, a prominent role in applications.

The *scalar case* is very well understood; historically the main examples appeared because of some extra property and preceded the development of a general theory of orthogonal polynomials by many decades. It is well known that the polynomials of Hermite, Laguerre and Jacobi are the only families orthogonal with respect to a positive measure on the real line which happen to have the following three extra properties: they are common eigenfunctions of some second order differential operator, they can be obtained using a Rodrigues formula, and the families obtained by taking their derivatives is once again a sequence of orthogonal polynomials. Each one of these characterizations is the result of a different effort, and they are usually associated to the names of to Bochner, Hildebrandt and Hahn, respectively. It follows that these three different properties are all equivalent, and in fact they can all be seen to follow from the so called Pearson equation. For a good historical account, see for instance [Ch,AS].

As one approaches the analogous problem for the *matrix valued case* it is only natural to take the large body of classical material reviewed above as a model.

We can now state the main thesis of this paper: the very well explored scalar case is a very poor guide to what is likely to happen in the largely unchartered matrix valued case. We mean this statement in two different ways: on the one hand there is the obvious fact

that dealing with *noncommuting* matrix coefficients for our polynomials produces all sorts of computational complications, on the other hand the richness brought about by this new situation has the consequence that many properties that were equivalent in the scalar case may no longer be so. In fact we will encounter phenomena that is entirely absent in the scalar case.

Due to the situation described above, this paper is more a "trail-blazing" effort than an attempt to give a neat collection of "theorem-proof" results. We feel that the subject is both rich and young enough to justify such an approach at this point.

We now move into part 2 of the introduction.

The paper [D2] starts the search for a matrix valued analog of the result of Bochner, see [B]. A large class of families of orthonormal matrix polynomials $(P_n)_n$, satisfying second-order differential equations of the form

$$P_n''(t)A_2(t) + P_n'(t)A_1(t) + P_n(t)A_0 = \Gamma_n P_n(t)$$
(1.1)

has recently been introduced in [DG1].

Here A_2 , A_1 and A_0 are matrix polynomials (which do not depend on n) of degrees less than or equal to 2, 1 and 0, respectively, and Γ_n are Hermitian matrices. As usual, the orthogonality of these families is with respect to a weight matrix W as introduced above. Another recent source of examples of this sort are the result of an independent effort, see [GPT1,GPT2,G].

Starting in [D2] one can see that when working with orthogonal matrix polynomials an important concept is that of scalar reducibility: we say that *W reduces to scalar weights* if there exists a nonsingular matrix *T* (independent of *t*) for which

$$W(t) = TD(t)T^*, (1.2)$$

with D(t) diagonal.

It is clear that the most interesting matrix examples are those nonreducible to scalar weights. In other words, an equivalence relation can be defined for weight matrices: W_1 is similar to W_2 if there exists a nonsingular matrix T (independent of t) such that $W_1 = TW_2T^*$. Weight matrices reducible to scalar weights are, precisely, those corresponding to the class of diagonal weights. Diagonal weights, as a collection of N scalar weights, belong to the study of scalar orthogonality more than to the matrix one.

We observe, however, that in [GPT2] one finds a notion of similarity for the *pair* consisting of the weight and the differential operator. This notion allows one to distinguish between certain situations that are considered equivalent under the present definition. See Example 5.1 in [GPT2]. As long as we are going to be concerned here with some of the other *extra properties* of matrix valued orthogonal polynomials, it is entirely appropriate to consider only the notion of similarity introduced in [D2].

The following example, which it is taken from [DG1], does not reduce to scalar weights, and its sequence of orthonormal matrix polynomials satisfies a second-order differential equation as (1.1):

$$W(t) = e^{-t^2} \begin{pmatrix} 1 + a^2 t^2 & at \\ at & 1 \end{pmatrix}.$$
 (1.3)

Now we meet the first instance of the important difference with respect to the scalar classical families of Jacobi, Laguerre and Hermite discussed above: the families introduced in [DG1] do not need to satisfy Rodrigues' formulas of the type

$$P_n(t) = C_n(\Phi^n W)^{(n)} W^{-1}, \quad n \geqslant 0, \tag{1.4}$$

where Φ is a matrix polynomial of degree not greater than 2 and C_n , $n \ge 0$, are nonsingular matrices. Instead, the sequence $(P_n)_n$ is shown to satisfy a *modified Rodrigues' formula*; for instance, the expression

$$P_n(t) = \left[e^{-t^2} \left(F(t) + \begin{pmatrix} a^2 n/2 & 0 \\ 0 & 0 \end{pmatrix} \right) \right]^{(n)} e^{t^2} F^{-1}(t), \tag{1.5}$$

where F is the matrix polynomial

$$F(t) = \begin{pmatrix} 1 + a^2 t^2 & at \\ at & 1 \end{pmatrix},$$

defines a sequence of orthogonal matrix polynomials with respect to the weight matrix (1.3). The example above is already given in [DG1]. For other structural formulas satisfied by this sequence of orthogonal polynomials see [DG2].

We will return later to the main result in [DG1], after we introduce other characters of our story.

By setting n=1, the scalar-type Rodrigues' formula gives the well-known Pearson equation:

$$(\Phi W)' = \Psi W, \tag{1.6}$$

where Ψ is a matrix polynomial of degree just 1 (the first orthogonal polynomial with respect to W). In the scalar case the converse is also true; moreover the Pearson equation for the weight w is equivalent to the fact that any sequence $(p_n)_n$ of orthogonal polynomials with respect to w satisfies a second-order differential equation

$$\phi p_n'' + \psi p_n' = \alpha_n p_n, \quad n \geqslant 0,$$

where ψ is a polynomial of degree 1 which does not depend on n. Notice that the polynomial ϕ , which appears in the Pearson equation for w, is also the coefficient of the second derivative of p_n .

To prove that a Pearson equation like (1.6) for the weight matrix W implies a scalar-type Rodrigues' formula for its sequence of orthogonal matrix polynomials, some commutativity conditions among Φ , Φ' , Φ'' and Ψ seem to be needed. We therefore assume that Φ is a scalar polynomial.

When the coefficients of Ψ commute with each other, the Pearson equation (1.6) can be explicitly integrated to get some examples of weight matrices W having orthogonal matrix polynomials satisfying a scalar-type Rodrigues' formula. Unfortunately, all these weight matrices reduce to scalar weights (see (1.2)). We will also include an example where we integrate the Pearson equation when the coefficients of Ψ do not commute, although once again this example reduces to scalar weights. However, something more interesting can be

done by considering a weaker condition than that of the positive definiteness of the weight matrix ((1) of Definition 1.1): in doing that we get some examples of orthogonal matrix polynomials which are relatives of the classical Bessel scalar polynomials.

Definition 1.2. We say that a $N \times N$ matrix of measures W supported on the real line is a (Hermitian) weight matrix if

- (1) W(A) is Hermitian for any Borel set $A \subset \mathbb{R}$;
- (2) W has finite moments of every order, and
- (3) $\int P(t) dW(t) P^*(t)$ is nonsingular whenever the leading coefficient of the matrix polynomial P is nonsingular.

Hermitian weight matrices are the analogs of signed measures in the scalar case. Before returning to the main result in [DG1] and its relevance to this paper we observe that the Pearson equation for *W* trivially implies the following second-order differential equation:

$$(\phi W)'' - (\Psi W)' = \theta.$$

Here θ denotes the null matrix.

According to [D2], this second-order differential equation implies a second-order differential equation for the orthogonal matrix polynomials with respect to *W*:

$$P_n''(t)\phi(t) + P_n'(t)\Psi(t) = \Gamma_n P_n(t).$$

It is worth noticing that the differential equation (1.1) satisfied by the orthogonal polynomials in the case of our example (1.3) is slightly different from the one above. In fact the coefficient A_0 which appears in (1.1) is essential to guarantee that the weight matrix (1.3) does not reduce to the scalar case.

This should allow us to understand why, in the matrix valued case, satisfying a scalar type Rodrigues' formula is no longer equivalent to satisfying a second-order differential equation like (1.1). Indeed, in [DG1], it is proved that the orthonormal matrix polynomials $(P_n)_n$ with respect to W satisfy a second-order differential equation as (1.1) if and only if $A_2W = WA_2^*$ and

$$(A_2(t)W(t))'' - (A_1(t)W(t))' + A_0W(t) = W(t)A_0^*,$$
(1.7)

as well as the extra condition that W satisfies the boundary conditions that

$$A_2(t)W(t)$$
 and $(A_2(t)W(t))' - A_1(t)W(t)$, (1.8)

should have vanishing limits at each of the endpoints of the support of W(t).

These conditions on *W* imply that a certain noncommutative Pearson equation has to be satisfied by the weight matrix *W*:

$$2(A_2(t)W(t))' = A_1(t)W(t) + W(t)A_1^*(t).$$
(1.9)

We emphasize that Eq. (1.9) does not imply the stronger one (1.7). In the scalar case both Eqs. (1.7) and (1.9) are equivalent (the second one being the Pearson equation). The noncommutativity of the matrix product implies that, in general, Eq. (1.9) also differs from

the scalar-type Pearson equation (1.6). Taking this into account, it is rather understandable that for orthogonal matrix polynomials the second order differential equation (such as (1.1)) does not imply scalar-type Rodrigues' formula (such as (1.4)).

We come now to part 3 of the introduction.

We prove, in Section 2, the equivalence between the Rodrigues' formula (1.4) for the orthogonal matrix polynomials $(P_n)_n$ and the Pearson equation for the weight matrix W, under the hypothesis that $\Phi(t) = \phi(t)I$, where ϕ is a scalar polynomial of degree not greater than 2.

In Section 3, we integrate the Pearson equation and show that assuming W to be positive definite, all the examples reduce to the scalar case. In Sections 4 and 5, we give however some generic examples of hermitian weight matrices satisfying a Pearson equation as in (1.6) which do not reduce to scalar weights.

Structural properties for the families introduced in Sections 4 and 5, where the weight matrix is no longer required to be positive definite, can be derived as in the case of the classical scalar families (so that we do not include them here). Section 6 gives further evidence of the strong differences between the scalar and the matrix case and should serve to further convince the reader of the relevance of the "trail-blazing" nature of this paper.

2. Pearson matrix equation and Rodrigues formula

As we mentioned in the introduction, the scalar-type Rodrigues' formula (1.4) for the orthogonal matrix polynomials $(P_n)_n$ with respect to the weight matrix W automatically implies the Pearson equation (1.6) for the weight matrix W: then, $\Psi = P_1$, the first orthogonal matrix polynomials with respect to W; this means that the leading coefficient of Ψ has to be nonsingular. To prove the converse, some commutativity conditions among Φ , Φ' , Φ'' and Ψ seem to be needed. We assume, as mentioned earlier, that $\Phi(t)$ is a scalar polynomial.

Theorem 2.1. Let W be a weight matrix satisfying the Pearson equation

$$(\phi(t)W)' = \Psi(t)W(t),$$

where $\phi(t)$ is a scalar polynomial of degree not greater than 2 and Ψ a matrix polynomial of degree 1 with nonsingular leading coefficient. We assume that the weight matrix W also satisfies the boundary conditions that $\phi(t)W(t)$ has vanishing limits at each of the endpoints of the support of W(t). If the degree of ϕ is 2 we assume, in addition, that its roots are different (just to avoid the analogs of the Bessel polynomials) and that the spectrum of the leading coefficient of Ψ is disjoint with the set of natural numbers \mathbb{N} . Then

$$P_n(t) = (\phi^n(t)W(t))^{(n)}W^{-1}(t)$$

is a sequence of matrix polynomials of degree n with non singular leading coefficients. Moreover, they are orthogonal with respect to W.

Proof. The orthogonality of the sequence follows easily using integration by parts. By a suitable linear change of variable we can assume that ϕ is equal to either 1, t, or $1 - t^2$ when its degree is 0, 1 or 2. We write $\Psi(t) = At + B$ with A nonsingular.

For $\phi = 1$, we can prove the result by using the formula

$$W^{(n)}W^{-1} = (W')^{(n-1)}W^{-1} = (\Psi W)^{(n-1)}W^{-1}$$
$$= (\Psi W^{(n-1)} + (n-1)AW^{(n-2)})W^{-1}$$

and complete induction on n.

For $\phi = t$, we use the formula

$$\begin{split} (t^k W)^{(n)} &= ((t^{k-1} t W)')^{(n-1)} W^{-1} \\ &= (k-1) (t^{k-1} W)^{(n-1)} W^{-1} + (t^{k-1} \Psi W)^{n-1} W^{-1} \\ &= [(k-1) (t^{k-1} W)^{(n-1)} + (At^k W)^{(n-1)} + (Bt^{k-1} W)^{(n-1)}] W^{-1} \\ &= [((k-1) I + B) (t^{k-1} W)^{(n-1)} + A (t^k W)^{(n-1)}] W^{-1} \end{split}$$

and induction on n to prove that $(t^k W)^{(n)} W^{-1}$ is a polynomial of degree k with nonsingular leading coefficient. The result then is just the case k = n.

For $\phi = 1 - t^2$, we use the formula

$$\begin{split} ((1-t^2)^k W)^{(n)} &= (((1-t^2)^{k-1}(1-t^2)W)')^{(n-1)}W^{-1} \\ &= [-2(k-1)(t(1-t^2)^{k-1}W)^{(n-1)} + ((1-t^2)^{k-1}\Psi W)^{n-1}]W^{-1} \\ &= [(-2(k-1)I + A)t(1-t^2)^{k-1}W)^{(n-1)} \\ &+ (B(1-t^2)^{k-1}W)^{(n-1)}]W^{-1} \\ &= \left[(-2(k-1)I + A)\left(t[(1-t^2)^{k-1}W]^{(n-1)} \right. \right. \\ &+ (n-1)[(1-t^2)^{k-1}W]^{(n-2)}\right) + B[(1-t^2)^{k-1}W]^{(n-1)} \right] W^{-1} \end{split}$$

and induction on n to prove that $[(1-t^2)^k W]^{(n)} W^{-1}$, $k \ge n$, is a polynomial of degree 2k-n with leading coefficient equal to

$$A_{k,n} = (-1)^{k+n} (A - (2k-2)I)(A - (2k-3)I) \cdots (A - (2k-(n+1))I).$$

The result follows now easily. \Box

3. Integrating the Pearson equation

In this section, we explicitly integrate the Pearson equation for the canonical values $\phi = 1$, $\phi(t) = t$ and $\phi(t) = (1 - t^2)$. This can be done easily as soon as we assume that the coefficients of the polynomial Ψ commute. Otherwise the integration of this first order matrix equation is not straightforward. Anyway, even in the case that the coefficients of Ψ do not commute, we conjecture that a weight matrix satisfying (1.6) will reduce to scalar weights; in fact, we include, at the end of this section, an example of this kind.

(1) When $\phi = 1$, we can write the Pearson equation (1.6) as

$$W'(t) = (2(B-I)t + A)W(t).$$

which can be solved explicitly when A and B commute to get

$$W(t) = e^{-t^2} e^{Bt^2 + At} C.$$

To avoid any integrability problem of W at ∞ , the real parts of the eigenvalues of B have to be less than 1.

(2) When $\phi = t$, we can write the Pearson equation (1.6) as

$$W'(t) = \left((A - I) + \frac{B + \alpha I}{t} \right) W(t),$$

which can be solved explicitly when A and B commute to get

$$W(t) = t^{\alpha} e^{-t} e^{At} t^B C.$$

To avoid any integrability problem of W at ∞ and at 0, the (real parts of the) eigenvalues of A have to be less than 1 and the (real parts of the) eigenvalues of B greater than $-\alpha - 1$, respectively.

(3) When $\phi = (1 - t)(1 + t)$, we can write the Pearson equation (1.6) as

$$W'(t) = \left(\frac{A + \alpha I}{1 + t} - \frac{B + \alpha I}{1 - t}\right) W(t),$$

which can be solved explicitly when A and B commute to get

$$W(t) = (1+t)^{\alpha} (1-t)^{\beta} (1+t)^{A} (1-t)^{B} C.$$

To avoid any integrability problem of W at ± 1 , the (real parts of the) eigenvalues of A have to be greater than $-\alpha - 1$ and the (real parts of the) eigenvalues of B greater than $-\beta - 1$, respectively.

Since the weight matrix W has to be Hermitian, in all the cases we have to impose, in addition to AB = BA, the conditions $BC = CB^*$ and $AC = CA^*$.

Unfortunately, when C is positive definite (that is W is a positive definite weight matrix), W reduces, in all the cases, to scalar weights (see 1.2). We prove it for $\phi(t) = 1$ (the rest of the cases can be proved analogously). Taking into account the conditions on the matrices A, B and C we can write

$$W(t) = e^{-t^2} e^{Bt^2 + At} C$$

= $e^{-t^2} C^{1/2} e^{C^{-1/2} (Bt^2 + At)C^{1/2}} C^{1/2}$

where $C^{-1/2}BC^{1/2}$ and $C^{-1/2}AC^{1/2}$ are now Hermitian commuting matrices; we can therefore take an unitary matrix U which simultaneous diagonalizes both matrices. Then, the weight can be written as

$$W(t) = e^{-t^2} C^{1/2} U e^{D_1 t^2 + D_2 t} U^* C^{1/2}.$$

with D_1 and D_2 diagonal matrices: that is, W reduces to scalar weights. This is the case for many examples of orthogonal matrix polynomials which can be found in the literature ([CMV,J1], for instance).

We complete this section integrating a particular Pearson equation where the coefficients of the polynomial Ψ do not commute:

We consider the Pearson equation

$$W'(t) = \left(\frac{A}{t} + \frac{B}{t-1}\right)W(t),\tag{3.1}$$

where the matrices A and B are given by

$$A = \frac{1}{2} \begin{pmatrix} 1-u \ u \\ 1-u \ u \end{pmatrix}, \quad B = \frac{1}{2} \begin{pmatrix} u & -u \\ u-2 \ -u+2 \end{pmatrix}, \quad u \in \mathbb{R}$$

(for convenience, we consider here $\phi = t(1-t)$ instead of $(1-t^2)$, although the example can be easily transformed to one corresponding to $(1-t^2)$).

Although the matrices A and B do not commute, we can integrate the Pearson equation (3.1) to get the solutions

$$W(t) = \left[\begin{pmatrix} 2u & -2u \\ -2 + 2u & -2u + 2 \end{pmatrix} + \sqrt{2} \begin{pmatrix} 1 - 2u & 2u \\ 1 - 2u & 2u \end{pmatrix} t^{1/2} + \begin{pmatrix} 0 & 0 \\ 2 & -2 \end{pmatrix} t \right] C.$$

If we look for a positive definite weight matrix W, a straightforward computation gives that C has to be of the form

$$C = \begin{pmatrix} a & a \\ a & b \end{pmatrix}, \quad b > a$$

and necessarily u = 0.

This gives for W the expression

$$W(t) = \begin{pmatrix} \sqrt{2}at^{1/2} & \sqrt{2}at^{1/2} \\ \sqrt{2}at^{1/2} & \sqrt{2}at^{1/2} + 2(1-t)(b-a) \end{pmatrix},$$

which can be factorized as

$$W(t) = \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 2(b-a)(1-t) & 0 \\ 0 & \sqrt{2}at^{1/2} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix}.$$

This shows that *W* reduces to scalar weights.

This example is very illustrative of what happens in the matrix case: there is a convenient choice of a positive definite matrix D so that the weight matrix

$$F(t) = W(t)DW^*(t)$$

is actually a positive definite matrix polynomial of degree 2. For this precise matrix D, the weight $t^{\alpha}(1-t)^{\beta}F$ satisfies not only a noncommutative Pearson equation like that of (1.9) (this happens for any choice of D) but more importantly also satisfies a second-order differential equation as that of (1.7). As a consequence the sequence of orthogonal matrix polynomials with respect to $t^{\alpha}(1-t)^{\beta}F$ satisfies a second order differential equation of the type (1.1). This weight matrix F does not reduce to scalar weights and it corresponds with the Example 5.2 of [GPT2].

4. Examples with A or B nilpotent

The construction above breaks down if C is Hermitian but not positive definite because then C does not have a Hermitian square root. In what follows we implicitly assume that C is nonsingular (otherwise condition (3) of Definition 1.2 is not fulfilled).

A number of consequences follow from the algebraic conditions imposed on A, B, C by the fact that W is Hermitian. For instance, if A or B are nilpotent, then C cannot be positive definite. Indeed, if for instance A is nilpotent of order k and $AC = CA^*$, it follows multiplying by A^{k-1} on the left and by $(A^*)^{k-2}$ on the right that $\theta = A^{k-1}C(A^*)^{k-1}$; since $A^{k-1} \neq \theta$, we deduce that C cannot be positive definite.

We give now some examples of this kind.

Take A and B the nilpotent matrices

$$A = \begin{pmatrix} 0 & u \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & v \\ 0 & 0 \end{pmatrix}.$$

The general expression for a Hermitian matrix C such that $AC = CA^*$ and $BC = CB^*$ is

$$C = \begin{pmatrix} a & b \\ b & 0 \end{pmatrix}.$$

(1) When $\phi = 1$, this gives for W the form

$$W(t) = e^{-t^2} \begin{pmatrix} 1 & ut \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & vt^2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a & b \\ b & 0 \end{pmatrix} = e^{-t^2} \begin{pmatrix} a + but + bvt^2 & b \\ b & 0 \end{pmatrix}.$$

A particular case of this example (a = v = 0, b = u = 1) can be found in [CMV].

(2) When $\phi = t$, this gives

$$W(t) = t^{\alpha} e^{-t} \begin{pmatrix} a + but + bv \log t & b \\ b & 0 \end{pmatrix}.$$

(3) Finally the case $\phi = (1 - t)(1 + t)$ gives the Hermitian weight matrix

$$W(t) = (1+t)^{\alpha} (1-t)^{\beta} \begin{pmatrix} a + bu \log(1+t) + bv \log(1-t) & b \\ b & 0 \end{pmatrix}.$$

5. Examples with A or B square root of a negative semidefinite matrix

If A or B are a square root of a negative semidefinite matrix, it follows easily that a matrix C such that $AC = CA^*$ (or $BC = CB^*$) cannot be positive definite.

Actually we can consider only upper triangular square roots of aI, $a \le 0$.

Indeed, take an orthonormal basis for which B^2 is diagonal with real entries and B is upper triangular. We prove by induction on N that then $B^2 = aI$, for certain $a \le 0$.

Indeed, for N = 2, it follows straightforwardly that under our hypothesis

$$B = \begin{pmatrix} a_{11} & a_{12} \\ 0 & -a_{11} \end{pmatrix},\tag{5.1}$$

so that $B^2 = a_{11}^2 I$.

Let us assume now that B has size N + 1. We split up the matrix B in blocks

$$B = \left(\begin{array}{cc} \tilde{B} & v \\ \theta & b \end{array} \right),$$

where \tilde{B} is an upper triangular matrix of size $N \times N$, v is a column vector of \mathbb{C}^N and $b \in \mathbb{C}$. Then

$$B^2 = \begin{pmatrix} \tilde{B}^2 & (\tilde{B} + aId.)v \\ \theta & b^2 \end{pmatrix}.$$

By the induction hypothesis, $\tilde{B}^2 = aI$, for certain $a \le 0$. This shows that the eigenvalues of \tilde{B} are $\pm \sqrt{a}$. Since B^2 is diagonal, we deduce that -b is an eigenvalue of \tilde{B} , and then also $B^2 = aI$.

All the upper triangular square roots of aI, $a \le 0$ can be generated recursively.

The case N = 2 has been already found (see (5.1) above).

For N = 3, we look for upper triangular matrices of the form

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & -a_{11} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix};$$

this gives two equations: the product of the second and first row (respectively) by the last column (in the general case of size N, we have N-1 equations: the product of the kth rows, $k=N-1,\ldots,1$, by the last column):

$$a_{23}(a_{33} - a_{11}) = 0,$$

 $a_{13}(a_{11} + a_{33}) + a_{12}a_{23} = 0.$

These equations (as well as those of the general case of size N) can be easily solved; in doing so, we find three different solutions (which cannot be reduced, in general, to lower size):

• $a_{23} = 0$, $a_{33} = -a_{11}$:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & -a_{11} & 0 \\ 0 & 0 & -a_{11} \end{pmatrix}.$$

• $a_{33} = a_{11} \neq 0$:

$$\begin{pmatrix} a_{11} & a_{12} & a_{12}a_{23}/(2a_{11}) \\ 0 & -a_{11} & a_{23} \\ 0 & 0 & a_{11} \end{pmatrix}.$$

• $a_{11} = a_{12} = 0$:

$$\begin{pmatrix} 0 & 0 & a_{13} \\ 0 & 0 & a_{23} \\ 0 & 0 & 0 \end{pmatrix}.$$

The corresponding Hermitian weight matrices can be computed by using that

$$x^{A} = \left(\cos\left(\sqrt{-a}\log x\right) - 1\right)I + \frac{A}{\sqrt{-a}}\sin\left(\sqrt{-a}\log x\right), \quad a < 0$$

and

$$x^A = I + A \log x, \quad a = 0.$$

The examples $e^{-t}t^AC$ are especially interesting. Indeed, from [DG1] it follows that the (positive definite) weight matrix

$$e^{-t}t^ABt^{A^*}$$

with $A^2 = aI$, $a \le 0$, and B positive definite, satisfies the second-order differential equation

$$(tW)''(t) + \left[(tI - 2A - I)W(t) \right]' - AW(t) = -W(t)A^*. \tag{5.2}$$

However, W does not satisfy the boundary conditions (1.8). Indeed, a simple calculation gives

$$(tW)' - A_1W = e^{-t}t^A(BA^* - AB)t^{A^*}.$$

The limit of this expression as t tends to 0^+ is θ if and only if $AB = BA^*$. That is not possible when B is positive definite but, as discussed above there exists B hermitian, so that $AB = BA^*$. For such a B the weight matrix $e^{-t}t^ABt^{A^*}$ reduces to $e^{-t}t^{2A}B$, that is, it is of the form considered above.

Since the weight matrix $W(t) = e^{-t}t^ABt^{A^*}$, B positive definite, does not satisfy the boundary conditions, the monic orthogonal matrix polynomials with respect to W do not satisfy the corresponding second-order differential equation

$$tP_n''(t) + P_n'(t)(2A + I - tI) - P_n(t)A = nP_n(t).$$

But taking B Hermitian with $AB = BA^*$, we have that the monic orthogonal matrix polynomials with respect to $e^{-t}t^ABt^{A^*}$ now satisfy the second-order differential equation

$$tP_n''(t) + P_n'(t)(2A + I - tI) = -nP_n(t).$$

6. Closing remarks

In this last section we strive to emphasize, once again, the basic fact that the scalar case is a very poor guide to the matrix valued situation.

If this is not already obvious from the considerations above we offer the following three items as further evidence. They illustrate slightly different aspects of a phenomenon that is completely absent in the scalar case.

(a) A look at [GPT1,GPT3] shows that in a special case of Jacobi polynomials of any size the space of second-order differential operators that has these polynomials as their common eigenfunctions is actually two dimensional. The two naturally appearing operators that

give a basis of this space are quite different in nature: one has a scalar valued leading coefficient of the form t(1-t)I while the other has a nonscalar leading coefficient. These two operators, and thus any pair of operators in the entire vector space, commute with each other.

- (b) A related phenomenon appears in [CG1], see (3.1) and (3.2). Here one finds a Chebychev-type family of matrix-valued orthogonal polynomials that satisfies two different first-order differential equations. In this case neither one of them has a scalar-valued leading coefficient. These two operators do not commute with each other.
- (c) As a final example we mention that in [CG2] one sees that for the Hermite-type polynomials introduced in [DG1], and further studied in [DG2], the space of second-order differential operators having them as common eigenfunctions has dimension four. This means that besides the equation given explicitly in [DG1], see (8.2), the monic orthogonal polynomials satisfy, for example, the equation

$$\begin{split} \hat{P}_{n}''(t) \frac{1}{\alpha^{2}} \begin{pmatrix} -\alpha t & (\alpha t - 1)(\alpha t + 1) \\ -1 & \alpha t \end{pmatrix} + \hat{P}_{n}'(t) \frac{1}{\alpha^{2}} \begin{pmatrix} -2\alpha & 2(\alpha^{2} + 2)t \\ 0 & 0 \end{pmatrix} \\ + \frac{1}{\alpha^{4}} \hat{P}_{n}(t) \begin{pmatrix} 0 & 2(\alpha^{2} + 2) \\ 4 & 0 \end{pmatrix} = \frac{1}{\alpha^{4}} \begin{pmatrix} 0 & (\alpha^{2} n + 2)(\alpha^{2} n + \alpha^{2} + 2) \\ 4 & 0 \end{pmatrix} \hat{P}_{n}(t). \end{split}$$

In this case some of these second-order differential operators commute with each other and some do not.

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