QBD processes and matrix valued orthogonal polynomials: some new explicit examples

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Abstract. The connection between birth-and-death processes and orthogonal polynomials was exploited starting with a paper in 1959 by Karlin and McGregor. At the end of their paper they discuss the case of a random walk on the set of all integers, and they compute its spectral matrix. This can be considered as a precursor to the connection between matrix valued orthogonal polynomials and QBD processes, recently discussed in the literature. We take a second look at this example of Karlin and McGregor and look at two variants of it. In each case we give an explicit expression for the spectral matrix. We try to include some pointers to the history of the subject.

Dedicated to Sam Karlin, who passed away on December 18, 2007.

1. Introduction

The recent paper [DRSZ], sets forth the advantage of using matrix valued orthogonal polynomials, as introduced by MG Krein back around 1950 in connection with QBD processes. For the same observation see also [G2] and the more recent paper [GI], where a rather sophisticated family of examples is displayed. The examples here are close to the one in the original paper by Karlin and McGregor.

As usual, a good idea has many parents, and this paper tries to show how the work of Karlin-McGregor, Krein and Berezans'ki can be seen as precursors of these interesting developments. As far as

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the natural development of this field, the original paper of Karlin and McGregor gives a good account of previous instances of the same kind of ideas in the work of W. Feller and H. P. McKean, jr. To these two authors one could add the contributions of I. J. Good, T. Harris, M. Kac, W. Ledermann and G. Reuter. For the benefit of the reader, these references are included in this paper. Apologies for those that are missing.

For a general guidance into the field of quasi-birth-and-death-processes (QBD) see [LPT], [LR1], [N].

I note that my interest in this field owes a lot to the work of S. Bochner, [B]. He was the Ph.D. advisor of S. Karlin who in turn was the advisor of M.F. Neuts, who is widely considered as responsible for the present interest in QBD processes. A small world indeed.

The plan for this paper is as follows:

1) We first review briefly the approach of S. Karlin and J. McGregor. This is done in section 2.
2) As a warmup we consider an explicit example of this representation, featuring Chebychev polynomials. This is done in section 3.
3) We introduce (with MG Krein) the notion of matrix valued orthogonal polynomials and introduce the notion of "folding the integers" to get as state space one that corresponds to a QBD with two phases. This idea of studying a difference operator on the integers by introducing a block difference operator on the non-negative integers is well discussed in the book by Berezans'ki, see [B1], which reports on the work started by his Ph.D. advisor MG Krein. This is done in section 4.
4) We revisit the example considered in the original paper of Karlin and McGregor of a random walk on the integers. The only extra result given here is an explicit expression of the matrix valued orthogonal polynomials associated to the spectral matrix already found back in 1959. This is done in section 5.
5) We modify the case treated by Karlin and McGregor to deal with attraction or repulsion towards the center located at 1/2. This is done in section 6.
6) We allow for a "defect at one site" in the previous model. This is done in section 7.

2. The Karlin-McGregor representation

If we have

$$\mathbb{P}_{i,j} = Pr\{X(n+1) = j | X(n) = i\}$$

for the 1-step transition probability of our Markov chain, and we put $p_i = \mathbb{P}_{i,i+1}$, $q_{i+1} = \mathbb{P}_{i+1,i}$, and $r_i = \mathbb{P}_{i,i}$ we get for the matrix $\mathbb{P}$, in the case of a birth and death process, the expression

$$\mathbb{P} = \begin{pmatrix} r_0 & p_0 & 0 & 0 & \\ q_1 & r_1 & p_1 & 0 & \\ 0 & q_2 & r_2 & p_2 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$

We will assume that $p_j > 0$, $q_{j+1} > 0$ and $r_j \geq 0$ for $j \geq 0$. We also assume $p_j + r_j + q_j = 1$ for $j \geq 1$ and by putting $p_0 + r_0 \leq 1$ we allow for the state $j = 0$ to be an absorbing state (with probability $1 - p_0 - r_0$). Some of these conditions can be relaxed.

If one introduces the polynomials $Q_j(x)$ by the conditions $Q_{-1}(0) = 0$, $Q_0(x) = 1$ and then using the notation

$$Q(x) = \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ \vdots \end{pmatrix}$$

we insist on the recursion relation

$$\mathbb{P}Q(x) = xQ(x)$$

one proves the existence of a unique measure $\psi(dx)$ supported in $[-1, 1]$ such that

$$\pi_j \int_{-1}^{1} Q_i(x)Q_j(x)\psi(dx) = \delta_{ij}$$

for suitable constants π_j, and one gets the Karlin-McGregor representation formula

$$(\mathbb{P}^n)_{ij} = \pi_j \int_{-1}^{1} x^n Q_i(x)Q_j(x)\psi(dx).$$

In general this representation is only of theoretical value, since the measure and the polynomials cannot be obtained explicitly. But, in the cases when the measure is known this gives a way to compute for a given pair i, j the value of the left handside from the knowledge of a finite piece of the matrix $\mathbb{P}$.

3. A Chebyshev type example

The example below illustrates nicely how certain recurrence properties of the process are related to the presence of point masses in the orthogonality measure. This is seen by comparing the two integrals at the end of the section.

Consider the matrix

$$\mathbb{P} = \begin{pmatrix} 0 & 1 & 0 & & & \\ q & 0 & p & & & \\ 0 & q & 0 & p & & \\ & & \ddots & \ddots & \ddots & \end{pmatrix}$$

with $0 \leq p \leq 1$ and $q = 1 - p$. We look for polynomials $Q_j(x)$ such that

$$Q_{-1}(x) = 0, \quad Q_0(x) = 1$$

and if $Q(x)$ denotes the vector

$$Q(x) \equiv \begin{pmatrix} Q_0(x) \\ Q_1(x) \\ Q_2(x) \\ \vdots \end{pmatrix}$$

we ask that we should have

$$\mathbb{P}Q(x) = xQ(x).$$

The matrix $\mathbb{P}$ can be conjugated into a symmetric one and in this fashion one can find the explicit expression for these polynomials.

We have

$$Q_j(x) = \left(\frac{q}{p}\right)^{j/2} \left[(2-2p)T_j\left(\frac{x}{2\sqrt{pq}}\right) + (2p-1)U_j\left(\frac{x}{2\sqrt{pq}}\right)\right]$$

where T_j and U_j are the Chebyshev polynomials of the first and second kind.

If $p \geq 1/2$ we have

$$\left(\frac{p}{1-p}\right)^n \int_{-\sqrt{4pq}}^{\sqrt{4pq}} Q_n(x)Q_m(x)\frac{\sqrt{4pq-x^2}}{1-x^2}dx = \delta_{nm}\begin{cases} 2(1-p)\pi, & n=0 \\ 2p(1-p)\pi, & n \geq 1 \end{cases}$$

while if $p \leq 1/2$ we get a new phenomenon, namely the presence of point masses in the spectral measure

$$\left(\frac{p}{1-p}\right)^n \left[\int_{-\sqrt{4pq}}^{\sqrt{4pq}} Q_n(x)Q_m(x)\frac{\sqrt{4pq-x^2}}{1-x^2}dx \right.$$
$$\left. + (2-4p)\pi[Q_n(1)Q_m(1) + Q_n(-1)Q_m(-1)]\right]$$
$$= \delta_{nm}\begin{cases} 2(1-p)\pi, & n=0 \\ 2p(1-p)\pi, & n \geq 1 \end{cases}$$

From a probabilistic point of view the interpretation of these two cases is very natural. People that prefer to avoid analytical tools and would rather think in terms of sample paths will be pleased.

4. Matrix valued orthogonal polynomials

Here we recall a notion due to M. G. Krein, see [K1, K2]. Given a self adjoint positive definite matrix valued smooth weight function $W(x)$ with finite moments, we can consider the skew symmetric bilinear form defined for any pair of matrix valued polynomial functions $P(x)$ and $Q(x)$ by the numerical matrix

$$(P, Q) = (P, Q)_W = \int_{\mathbb{R}} P(x)W(x)Q^*(x)dx,$$

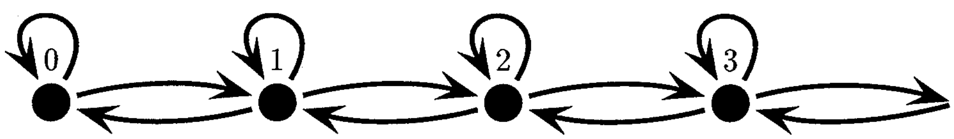
where $Q^*(x)$ denotes the conjugate transpose of $Q(x)$. By the usual construction this leads to the existence of a sequence of matrix valued orthogonal polynomials with non singular leading coefficient.

Given an orthogonal sequence $\{P_n(x)\}_{n\geq 0}$ one gets by the usual argument a three term recursion relation

$$xP_n(x) = A_nP_{n-1}(x) + B_nP_n(x) + C_nP_{n+1}(x), \quad (1)$$

where A_n, B_n and C_n are matrices and the last one is nonsingular.

In the case of a birth and death process it is useful to think of a graph like

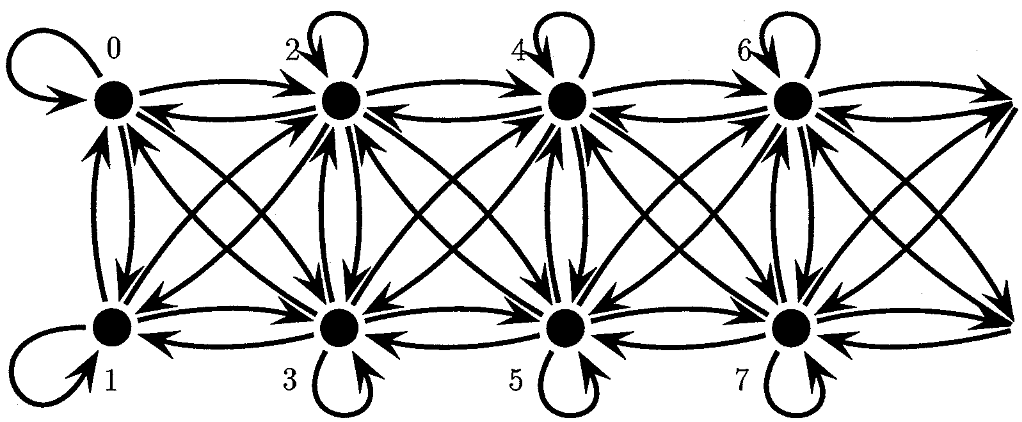


If we want to deal with a nearest neighbourhood random walk on the set of all integers it is convenient to fold the integers to get a two stranded version of the nonnegative integers. This is a very useful and classical idea which plays an important role in [B1] and can be seen used in the continuous case in [T]. The resulting state space is the one that corresponds to a QBD process with two phases.

The labelling in the graph below is such that the nonnegative integers $0, 1, 2, 3, ...$ correspond to the upper strand on the graph and are labelled $0, 2, 4, 6, ...$ while the original states $-1, -2, -3, ...$ are mapped onto $1, 3, 5, ...$

This idea can be pushed further.

The graph below



clearly corresponds to a general block tridiagonal matrix, with blocks of size 2×2. The transitions here are much more general than those needed in the examples to be given later. In particular all the diagonal transitions between states on the two strands as well as the self-loops are set to zero.

For the general graph above if $\mathbb{P}_{i,j}$ denotes the i, j block of $\mathbb{P}$ we can generate a sequence of 2×2 matrix valued polynomials $Q_i(t)$ by imposing the three term recursion (1) of this section. By using the notation of section 2, we would have

$$\mathbb{P}Q(x) = xQ(x)$$

where the entries of the column vector $Q(x)$ are now 2×2 matrices.

Proceeding as in the scalar case, this relation can be iterated to give

$$\mathbb{P}^n Q(x) = x^n Q(x)$$

and if we assume the existence of a weight matrix $W(x)$ as in section 2, with the property

$$(Q_j, Q_j)\delta_{i,j} = \int_{\mathbb{R}} Q_i(x)W(x)Q_j^*(x)dx,$$

it is then clear that one can get an expression for the (i, j) entry of the block matrix $\mathbb{P}^n$ that would look exactly as in the scalar case, namely

$$(\mathbb{P}^n)_{ij}(Q_j, Q_j) = \int x^n Q_i(x) W(x) Q_j^*(x) dx.$$

Just as in the scalar case, this expression becomes useful when we can get our hands on the matrix valued polynomials $Q_i(x)$ and the orthogonality measure $W(x)$. Notice that we have not discussed conditions on the matrix $\mathbb{P}$ to give rise to such a measure.

In summary the spectral theory of a scalar double-infinite tridiagonal matrix leads naturally to a 2×2 semi-infinite matrix. This has been looked at in terms of random walks in [P]. In [ILMV], this work is elaborated further to get a formula that could be massaged to look like the right hand side of the one above.

5. The example in Karlin-McGregor

The probabilities of going right or left are p and q, respectively, with $p + q = 1$.

The block tridiagonal matrix $\mathbb{P}$ is given by

$$\mathbb{P} = \begin{pmatrix} 0 & q & p & 0 & 0 & 0 & \dots & \dots & \dots \\ p & 0 & 0 & q & 0 & 0 & \dots & \dots & \dots \\ q & 0 & 0 & 0 & p & 0 & \dots & \dots & \dots \\ 0 & p & 0 & 0 & 0 & q & \dots & \dots & \dots \\ 0 & 0 & q & 0 & 0 & 0 & p & 0 & \dots \\ 0 & 0 & 0 & p & 0 & 0 & 0 & q & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

Here is the weight matrix, which was already computed by Karlin and McGregor:

In the interval $|x| \leq \sqrt{4pq}$

$$\frac{1}{\sqrt{4pq - x^2}} \begin{pmatrix} 1 & x/2q \\ x/2q & p/q \end{pmatrix}$$

In this example we have,

$$B_0 = \begin{pmatrix} 0 & q \\ p & 0 \end{pmatrix}, \quad B_k = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \ k \geq 1$$

we also have

$$A_k = \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix}, k \geq 1$$

and

$$C_k = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}, k \geq 0$$

The orthogonal polynomials given by

$$A_k P_{k-1}(x) + B_k P_k(x) + C_k P_{k+1}(x) = x P_k(x)$$

with $P_{-1}(x) = 0, P_0(x) = I$, can be readily expressed in terms of Chebyshev polynomials.

Let us denote by $U_n(x)$ the Chebyshev polynomials of the second kind, which satisfy

$$U_{n+1}(x) + U_{n-1}(x) = 2xU_n(x), \quad \text{with} \quad U_{-1}(x) = 0 \quad \text{and} \quad U_0(x) = 1.$$

The relation with the Chebyshev polynomials $U_n(x)$, is given by

$$P_k(x) = \begin{pmatrix} (q/p)^{k/2} U_k(x^*) & -(q/p)^{(k+1)/2} U_{k-1}(x^*) \\ -(p/q)^{(k+1)/2} U_{k-1}(x^*) & (p/q)^{k/2} U_k(x^*) \end{pmatrix}$$

with $x^* = x/(2\sqrt{pq})$.

A couple of extra historical comments: this model is treated in the Ph.D. thesis of W. Pruitt, see [P] but there is no use there of the spectral matrix that had been found earlier. The advantage of using this matrix is pointed out in [ILMV].

6. An attractive or repulsive force

Consider now a modification of the example in Karlin-McGregor with probabilities p of going away from the center (located at 1/2) and q of going towards the center.

This yields the matrix

$$\mathbb{P} = \begin{pmatrix} 0 & q & p & 0 & \dots & \dots & \dots & \dots & \dots \\ q & 0 & 0 & p & \dots & \dots & \dots & \dots & \dots \\ q & 0 & 0 & 0 & p & 0 & \dots & \dots & \dots \\ 0 & q & 0 & 0 & 0 & p & \dots & \dots & \dots \\ 0 & 0 & q & 0 & 0 & 0 & p & 0 & \dots \\ 0 & 0 & 0 & q & 0 & 0 & 0 & p & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

with $p + q = 1$.

The corresponding weight matrix is given below:

In the interval $|x| \leq \sqrt{4pq}$

$$\frac{\sqrt{4pq - x^2}}{1 - x^2} \begin{pmatrix} 1 & x \\ x & 1 \end{pmatrix}$$

and if $p < 1/2$ one adds the "point masses"

$$(1-2p)\pi\left[\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\delta_{-1}+\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\delta_1\right]$$

One more historical note:

E. Schroedinger himself, see [SchK], considered the problem of a discrete harmonic oscillator. In that case there is a quadratic potential resulting in a linear attractive force. The stochastic model considered above can be seen as a variant of this where the potential is given by a scalar multiple of the function "distance to the origin" resulting in a force that is a constant multiple of the sign function. This results in a standard random walk which feels the presence of this extra force. We have not found a classical treatment of the continuous quantum mechanical version of this problem in the literature, although it is likely that it is written up somewhere in terms of appropriate linear combinations of Airy functions.

7. Allowing for one defect

The example of random walk on the integers given originally in Karlin-McGregor can be modified even further by allowing a "defect" at one site, so that the one step transition probability matrix looks like

$$\mathbb{P}=\begin{pmatrix}
0 & x_2 & x_1 & 0 & \dots & \dots & \dots & \dots & \dots\\
q & 0 & 0 & p & \dots & \dots & \dots & \dots & \dots\\
q & 0 & 0 & 0 & p & 0 & \dots & \dots & \dots\\
0 & q & 0 & 0 & 0 & p & \dots & \dots & \dots\\
0 & 0 & q & 0 & 0 & 0 & p & 0 & \dots\\
0 & 0 & 0 & q & 0 & 0 & 0 & p & \dots\\
\dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots
\end{pmatrix}$$

with $x_1 + x_2 = 1$.

The new weight matrix is now:

In the interval $|x| \le \sqrt{4pq}$

$$W=\frac{\sqrt{4pq-x^2}}{1-x^2}\begin{pmatrix}p(1-x_1) & p(1-x_1)x\\ p(1-x_1)x & (1-p)x_1+(p-x_1)x^2\end{pmatrix}$$

Notice that if $x_1 = p$ this matrix is a scalar multiple of the one in the previous example, as it should be.

If $p < 1/2$ one needs to add "point masses"

$$(1-x_1)(1-2p)\pi\left[\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\delta_{-1}+\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\delta_1\right].$$

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