Stochastic Darboux transformations for quasi-birth-and-death processes and urn models ☆

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We consider stochastic UL and LU block factorizations of the one-step transition probability matrix for a discrete-time quasi-birth-and-death process, namely a stochastic block tridiagonal matrix. The simpler case of random walks with only nearest neighbors transitions gives a unique LU factorization and a one-parameter family of factorizations in the UL case. The block structure considered here yields many more possible factorizations resulting in a much enlarged class of potential applications. By reversing the order of the factors (also known as a Darboux transformation) we get new families of quasi-birth-and-death processes where it is possible to identify the matrix-valued spectral measures in terms of a Geronimus (UL) or a Christoffel (LU) transformation of the original one. We apply our results to one example going with matrix-valued Jacobi polynomials arising in group representation theory. We also give urn models for some particular cases.

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1. Introduction

Among the class of Markov chains there is one set that can be analyzed by so-called "spectral methods", namely random walks (discrete-time) and birth-and-death processes (continuous time). They go with a one-step tridiagonal matrix and this naturally leads to a self-adjoint operator in certain Hilbert space. Starting with [16–18], and using earlier ideas of W. Feller and H. P. McKean in the case of diffusion processes, there is a vast literature on this subject, which relies on the rich theory of orthogonal polynomials. A historical overview of this material can be seen, for instance, in [15]. Eventually this approach was extended to cover so-called quasi-birth-and-death (QBD) processes by exploiting matrix-valued orthogonal polynomials, a notion due to M.G. Kreĭn, see [19,20] for this, and [2,6] for its use in the study of QBD

processes. Here the tridiagonal matrix is replaced by a block tridiagonal one. For a general reference about QBD processes see [21,23]. The spectral methods work well when one has knowledge of the orthogonal polynomials and the spectral measure associated with the one-step transition probability matrix. Needless to say, this is a limitation on the wide practical use of the method, although many interesting general results are available.

On the other hand, given either a tridiagonal or a block tridiagonal matrix, assumed here to be stochastic, a natural problem is to explicitly construct some simple probabilistic model (such as an urn model) whose one-step transition probability matrix coincides with the given one. This is not as simple as it may sound: to give an instance of this consider the case of the matrices corresponding to the Krawtchouk and the Hahn orthogonal polynomials. In these two cases the urn model predates the consideration of the spectral problem for the tridiagonal matrices by a long stretch, see for instance [6] or [5], p. 378, where one sees the connection with work of P. and T. Ehrenfest in 1907 (see [4]), as well as D. Bernoulli (1769) and S. Laplace (1812). Both of these cases are very special cases of the so-called Askey-Wilson tridiagonal matrices, see [1], for which nobody has been able to find a nice urn model. For another well known example of a tridiagonal matrix, namely the one associated to the Jacobi polynomials, a first and rather contrived urn model was only given, as far as we know, in [7] (see also [10] for a different urn model). For a matrix-valued version of the Jacobi polynomials a pair of explicit models was given in [13].

Keeping in mind the two points raised above, we are in a position to describe the purpose of this paper. Extending our previous work for random walks in [10], we consider the block tridiagonal transition probability matrix of a discrete-time QBD process and perform UL and LU stochastic block factorizations. Unlike the case of random walks, where the UL factorization comes with exactly one free parameter, now, for the stochastic block factorization, there may be many degrees of freedom, as we will see in Section 2. The same applies for the LU factorization. The main motivation of this factorization is to analyze the urn model associated with the QBD process in terms of two unrelated and simpler urn models and to combine them to obtain a simpler description of the original QBD process.

Once we are able to perform UL and LU stochastic block factorizations of the block tridiagonal transition probability matrix of a discrete-time QBD process, we will give a general way to produce a family of new ones, performing what is called a discrete Darboux transformation by reversing the order of multiplication (see Section 3). We will also give a way to relate the original and the new spectral ingredients, i.e. the matrix-valued orthogonal polynomials and the matrix-valued spectral measure.

We apply our results in Section 4 to study one example of Jacobi type coming from group representation theory, introduced for the first time in [12] (see also [13]). We focus on the 2×2 case and study two particular situations, where we can illustrate the features that arise in the case of a general QBD process. Finally, in Section 5, we start from a special case of the urn model described in [13] and find a different urn model as an application of the method of the stochastic block factorization.

2. Stochastic LU and UL block factorization

Let P be the one-step transition probability matrix of a discrete-time quasi-birth-and-death (QBD) process with state space $\mathbb{Z}_{\geq 0} \times \{1, 2, \ldots, d\}$, $d \geq 1$, given by

$$
P = \begin{pmatrix}
B_0 & A_0 & 0 & \\
C_1 & B_1 & A_1 & \\
0 & C_2 & B_2 & A_2 \\
& & \ddots & \ddots & \ddots
\end{pmatrix}.
\tag{2.1}
$$

Here A_n, B_n and C_n are $d \times d$ matrices. We will assume for simplicity that the matrices A_n and C_n are nonsingular. The symbol 0 as well as all the unfilled entries in (2.1) stand for the $d \times d$ block zero matrix. When $d = 1$ we recover the classical random walk with state space $\mathbb{Z}_{\geq 0}$.

Let us denote by e_j the j-th canonical d-dimensional vector and $\boldsymbol{e}_d$ the d-dimensional vector with all components equal to 1, i.e.

$$\boldsymbol{e}_d = (1, 1, \ldots, 1)^T.$$

Since P is a stochastic matrix, we have nonnegative (scalar) entries, i.e.

$$e_i^T A_n e_j \geq 0, \quad e_i^T B_n e_j \geq 0, \quad e_i^T C_{n+1} e_j \geq 0, \quad i, j = 1, \ldots, d, \quad n \geq 0,$$

and all (scalar) rows add up to one, i.e.

$$(B_0 + A_0)\boldsymbol{e}_d = \boldsymbol{e}_d, \quad (C_n + B_n + A_n)\boldsymbol{e}_d = \boldsymbol{e}_d, \quad n \geq 1.$$

Observe that all block entries of P are *semi-stochastic* $d \times d$ matrices, i.e. all entries are nonnegative and $A_n\boldsymbol{e}_d \leq \boldsymbol{e}_d$, $B_n\boldsymbol{e}_d \leq \boldsymbol{e}_d$ and $C_{n+1}\boldsymbol{e}_d \leq \boldsymbol{e}_d$ for $n \geq 0$ (component wise).

A diagram of the transitions between states looks as follows (for $d = 2$):
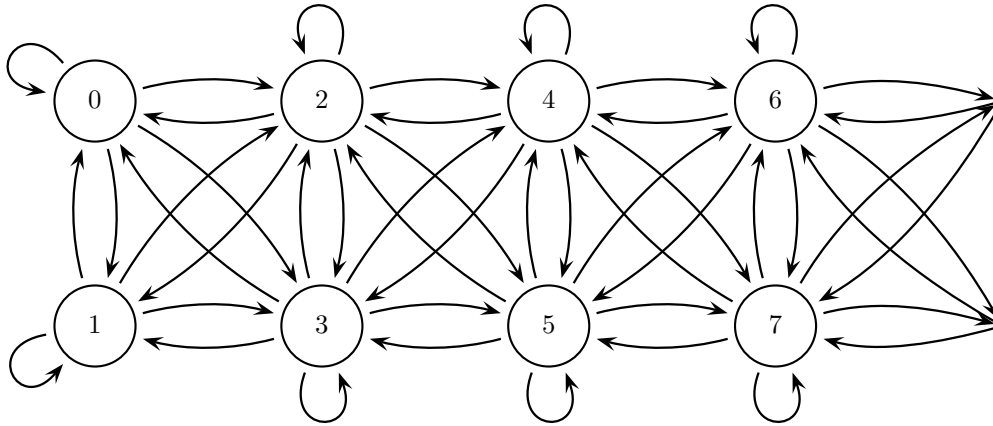
It will turn out to be useful to perform a UL block factorization of the matrix P in the following way

$$P = \begin{pmatrix} B_0 & A_0 & \\ C_1 & B_1 & A_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} Y_0 & X_0 & \\ 0 & Y_1 & X_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} S_0 & 0 & \\ R_1 & S_1 & 0 \\ & \ddots & \ddots & \ddots \end{pmatrix} = P_U P_L, \qquad (2.2)$$

with the condition that P_U and P_L *are also stochastic matrices*, i.e. all (scalar) entries are nonnegative and

$$(X_n + Y_n)\boldsymbol{e}_d = \boldsymbol{e}_d, \quad n \geq 0, \quad S_0\boldsymbol{e}_d = \boldsymbol{e}_d, \quad (R_n + S_n)\boldsymbol{e}_d = \boldsymbol{e}_d, \quad n \geq 1. \qquad (2.3)$$

Observe that S_0 must be stochastic, while the rest of the block entries of P_U and P_L must be semi-stochastic. A direct computation shows that

$$\begin{aligned} A_n &= X_n S_{n+1}, \quad n \geq 0, \\ B_n &= X_n R_{n+1} + Y_n S_n, \quad n \geq 0, \\ C_n &= Y_n R_n \quad n \geq 1. \end{aligned} \qquad (2.4)$$

Since A_n and C_n are nonsingular then X_n, Y_n, R_{n+1} and $S_{n+1}, n \geq 0$, are nonsingular matrices. S_0 may or may not be nonsingular. This factorization, just as in the scalar situation (see [10]), simplifies the

interpretation of the original QBD process P, expressing it as the composition of two simpler QBD processes, P_U and P_L.

One could have performed the factorization the other way around in the form

$$P = \begin{pmatrix} B_0 & A_0 & \\ C_1 & B_1 & A_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} \widetilde{S}_0 & 0 & \\ \widetilde{R}_1 & \widetilde{S}_1 & 0 \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \widetilde{Y}_0 & \widetilde{X}_0 & \\ 0 & \widetilde{Y}_1 & \widetilde{X}_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} = \widetilde{P}_L \widetilde{P}_U, \tag{2.5}$$

in which case we have a LU block factorization with relations

$$A_n = \widetilde{S}_n \widetilde{X}_n, \quad n \geq 0,$$
$$B_n = \widetilde{R}_n \widetilde{X}_{n-1} + \widetilde{S}_n \widetilde{Y}_n, \quad n \geq 0,$$
$$C_n = \widetilde{R}_n \widetilde{Y}_{n-1} \quad n \geq 1.$$

As we will see the LU block factorization will have *fewer* degrees of freedom than the UL block factorization.

Let us focus first on the UL block factorization (2.2). We remark here an important difference with respect to the scalar situation (see [10]). In the scalar situation the UL factorization has exactly one free parameter y_0 (defined below), while in the LU factorization case the factorization is unique. This is *not the case* for the UL and LU block factorizations, where there may be many degrees of freedom. For instance, in the scalar situation, where we use lower case symbols, one could compute x_n and r_{n+1} in terms of y_n and s_{n+1}, respectively, for $n \geq 0$, since both factors P_U and P_L must be stochastic matrices. Then $x_n = 1 - y_n, r_{n+1} = 1 - s_{n+1}, n \geq 0$, and $s_0 = 1$, i.e. all entries of P_U and P_L can be computed in terms of only one free parameter, y_0 (see Lemma 2.2 of [10]).

The stochasticity conditions on P_U and P_L gives the relations (2.3), but we notice that it is not possible to compute, for instance, all entries of S_0 by having only the information that $S_0 e_d = e_d$. The same is true for the rest of coefficients, i.e. we can not compute all entries of X_n in terms of Y_n from the information that $(X_n + Y_n) e_d = e_d$ (same for R_n and S_n).

One way of computing the block entries X_n, Y_n, R_n, S_n comes directly from (2.4). From the first and third relation we can compute $S_n, R_n, n \geq 1$ in terms of $X_n, n \geq 0$ and $Y_n, n \geq 1$, respectively. The second relation gives then

$$Y_{n+1} = C_{n+1} \left(B_n - Y_n X_{n-1}^{-1} A_{n-1} \right)^{-1} X_n, \quad n \geq 1, \quad \text{and} \quad Y_1 = C_1 \left(B_0 - Y_0 S_0 \right)^{-1} X_0.$$

Therefore, all coefficients can be computed in terms of Y_0, S_0 and $X_n, n \geq 0$. We will see below that all these inverses are well defined as long as certain invertibility conditions are satisfied. Apart from this we have to impose certain positivity conditions on all entries of X_n, Y_n, R_n, S_n. This gives an infinite number of free parameters in general and it is very difficult to pick a "natural one" among the possible solutions.

We propose now one way of computing the block entries X_n, Y_n, S_n, R_n using what corresponds to the "monic" version of P in connection with matrix-valued polynomials, see [19,20]. This method was used, for a different purpose, in [8]. Let us call

$$L_n = (A_0 \cdots A_{n-1})^{-1}, \quad n \geq 1, \quad L_0 = I. \tag{2.6}$$

Observe that all L_n are invertible, by assumption, and $L_n L_{n+1}^{-1} = A_n$. Then we have

$$P = LJL^{-1}, \tag{2.7}$$

where

$$L = \begin{pmatrix} L_0 & & \\ & L_1 & \\ & & \ddots \end{pmatrix}, \quad J = \begin{pmatrix} \widehat{B}_0 & I & \\ \widehat{C}_1 & \widehat{B}_1 & I & \\ & \ddots & \ddots & \ddots \end{pmatrix}.$$

The "monic" block entries $\widehat{B}_n$ and $\widehat{C}_n$ are related to the old ones by the relations

$$\widehat{B}_n = L_n^{-1} B_n L_n, \quad n \geq 0, \qquad \widehat{C}_n = L_n^{-1} C_n L_{n-1} = L_n^{-1} C_n A_{n-1} L_n, \quad n \geq 1.$$

Consider now the UL block factorization of the "monic" operator J in the following way

$$J = \begin{pmatrix} \widehat{B}_0 & I & \\ \widehat{C}_1 & \widehat{B}_1 & I & \\ & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} \alpha_0 & I & \\ 0 & \alpha_1 & I & \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} I & 0 & \\ \beta_1 & I & 0 & \\ & \ddots & \ddots & \ddots \end{pmatrix} = \boldsymbol{\alpha}\boldsymbol{\beta}. \tag{2.8}$$

Then we have

$$\widehat{B}_n = \beta_{n+1} + \alpha_n, \quad n \geq 0, \tag{2.9}$$
$$\widehat{C}_n = \alpha_n \beta_n, \quad n \geq 1.$$

These relations give a direct way to compute α_n and β_n in terms of $\widehat{B}_n$, $\widehat{C}_n$ and a *free matrix-valued parameter* α_0. Indeed, the first terms are given recursively by

$$\beta_1 = \widehat{B}_0 - \alpha_0, \qquad\qquad \alpha_1 = \widehat{C}_1(\widehat{B}_0 - \alpha_0)^{-1}$$
$$\beta_2 = \widehat{B}_1 - \widehat{C}_1(\widehat{B}_0 - \alpha_0)^{-1}, \qquad \alpha_2 = \widehat{C}_2\left[\widehat{B}_1 - \widehat{C}_1(\widehat{B}_0 - \alpha_0)^{-1}\right]^{-1}, \quad \text{etc.}$$

Observe from (2.9), and since $\widehat{C}_n$ is a nonsingular matrix, that α_n, β_n must be nonsingular matrices as well. This means that the free parameter α_0 is subject to certain invertibility conditions, i.e. $\widehat{B}_0 - \alpha_0, \widehat{B}_1 - \widehat{C}_1(\widehat{B}_0 - \alpha_0)^{-1}$, etc, must be nonsingular matrices.

Substituting (2.8) into (2.7) leads to

$$P = [L\boldsymbol{\alpha}]\left[\boldsymbol{\beta}L^{-1}\right],$$

which is a UL factorization of P. In general, this factorization will not give stochastic factors as in (2.2). To guarantee this we will need to introduce below more degrees of freedom while keeping the UL structure. Let us denote by T the block diagonal invertible matrix

$$T = \begin{pmatrix} \tau_0 & & \\ & \tau_1 & \\ & & \ddots \end{pmatrix}.$$

Then we can write P as

$$P = [L\boldsymbol{\alpha}T]\left[T^{-1}\boldsymbol{\beta}L^{-1}\right] = P_U P_L.$$

Identifying block entries with (2.2) we get

$$X_n = L_n \tau_{n+1}, \quad Y_n = L_n \alpha_n \tau_n, \quad n \geq 0, \tag{2.10}$$
$$S_n = \tau_n^{-1} L_n^{-1}, \quad R_{n+1} = \tau_{n+1}^{-1} \beta_{n+1} L_n^{-1}, \quad n \geq 0.$$

Relations (2.3) give

$$L_n(\alpha_n\tau_n + \tau_{n+1})\boldsymbol{e}_d = \boldsymbol{e}_d, \quad n \geq 0 \tag{2.11}$$

$$(\beta_{n+1}L_n^{-1} + L_{n+1}^{-1})\boldsymbol{e}_d = \tau_{n+1}\boldsymbol{e}_d, \quad n \geq 0, \tag{2.12}$$

$$\tau_0^{-1}\boldsymbol{e}_d = \boldsymbol{e}_d. \tag{2.13}$$

If (2.12) and (2.13) hold, then (2.11) must hold as well. Indeed, for $n = 0$, we have

$$(\alpha_0\tau_0 + \tau_1)\boldsymbol{e}_d = (\alpha_0 + \beta_1 + L_1^{-1})\boldsymbol{e}_d = (B_0 + A_0)\boldsymbol{e}_d = \boldsymbol{e}_d,$$

while for $n \geq 1$, we have

$$
\begin{aligned}
L_n(\alpha_n\tau_n + \tau_{n+1})\boldsymbol{e}_d &= \left[L_n\alpha_n(\beta_nL_{n-1}^{-1} + L_n^{-1}) + L_n(\beta_{n+1}L_n^{-1} + L_{n+1}^{-1})\right]\boldsymbol{e}_d \\
&= \left[L_n\alpha_n\beta_nL_{n-1}^{-1} + L_n\alpha_nL_n^{-1} + L_n\beta_{n+1}L_n^{-1} + L_nL_{n+1}^{-1}\right]\boldsymbol{e}_d \\
&= \left[C_n + B_n + A_n\right]\boldsymbol{e}_d = \boldsymbol{e}_d.
\end{aligned}
$$

Observe that (2.12) gives one way to compute τ_n which may allow for several degrees of freedom as well. Computing τ_n using (2.12) and (2.13) does not yet guarantee that P_U and P_L are going to be stochastic. We must still verify the positivity of the entries.

Using (2.10) and the explicit expression of α_n, β_n, we have that

$$X_n = (A_0 \cdots A_{n-1})^{-1}\tau_{n+1}, \quad S_n = \tau_n^{-1}A_0 \cdots A_{n-1}, \quad n \geq 0, \quad Y_0 = \alpha_0\tau_0,$$

and

$$
\begin{aligned}
R_1 &= \tau_1^{-1}(B_0 - \alpha_0), & Y_1 &= C_1(B_0 - \alpha_0)^{-1}\tau_1, \\
R_2 &= \tau_2^{-1}A_0(B_1 - C_1(B_0 - \alpha_0)^{-1}A_0), & Y_2 &= C_2[B_1 - C_1(B_0 - \alpha_0)^{-1}A_0]^{-1}A_0^{-1}\tau_2, \quad \text{etc.}
\end{aligned}
$$

Therefore, if we are able to propose a good candidate for τ_n, then we can compute all block entries X_n, Y_n, R_n, S_n in terms of only $Y_0 = \alpha_0\tau_0$.

Remark 2.1. In general, there are few conclusions we can derive for the sequence τ_n in terms of the positivity of the block entries X_n, Y_n, R_n, S_n. In particular, since $S_0 = \tau_0^{-1}$, then τ_0^{-1}, (but not necessarily τ_0) must be a stochastic matrix. Also from $X_0 = \tau_1$ and $Y_0 = \alpha_0\tau_0$ we must have that τ_1 and $\alpha_0\tau_0$ are semi-stochastic. In particular, since $\alpha_0 = Y_0\tau_0^{-1}$ and τ_0^{-1} is stochastic, then α_0 must be at least semi-stochastic as well.

Similar considerations apply if we consider the LU block factorization (2.5). Indeed, we will have

$$P = \left[L\widetilde{\beta}\widetilde{T}\right]\left[\widetilde{T}^{-1}\widetilde{\boldsymbol{\alpha}}L^{-1}\right] = \widetilde{P}_L\widetilde{P}_U,$$

where now the coefficients $\widetilde{\alpha}_n, \widetilde{\beta}_n$ can be computed by

$$
\begin{aligned}
\widehat{B}_n &= \widetilde{\beta}_n + \widetilde{\alpha}_n, \quad n \geq 0, \\
\widehat{C}_n &= \widetilde{\beta}_n\widetilde{\alpha}_{n-1}, \quad n \geq 1.
\end{aligned}
$$

Identifying block entries with (2.5) we get

$$\widetilde{X}_n = \widetilde{\tau}_n^{-1} L_{n+1}^{-1}, \quad \widetilde{Y}_n = \widetilde{\tau}_n^{-1} \widetilde{\alpha}_n L_n^{-1}, \quad n \geq 0, \tag{2.14}$$
$$\widetilde{S}_n = L_n \widetilde{\tau}_n, \quad \widetilde{R}_{n+1} = L_{n+1} \widetilde{\beta}_{n+1} \widetilde{\tau}_n, \quad n \geq 0.$$

In this case we will get the relations

$$L_n (\widetilde{\beta}_n \widetilde{\tau}_{n-1} + \widetilde{\tau}_n) \boldsymbol{e}_d = \boldsymbol{e}_d, \quad n \geq 0,$$
$$(\widetilde{\alpha}_n L_n^{-1} + L_{n+1}^{-1}) \boldsymbol{e}_d = \widetilde{\tau}_n \boldsymbol{e}_d, \quad n \geq 0.$$

Observe now that $\widetilde{\tau}_0$ must be stochastic ($\widetilde{\beta}_0 = 0$). This factorization will only depend on the sequence $\widetilde{\tau}_n$, since the sequences $\widetilde{\alpha}_n$ and $\widetilde{\beta}_n$ are uniquely determined in this case.

3. Stochastic block Darboux transformations

Assume that using the strategy above we have found appropriately α_0 and τ_n such that P_U and P_L are stochastic matrices. We can perform what is called a *discrete Darboux transformation* by reversing the order of multiplication. The Darboux transformation for second-order differential operators has a long history but probably the first reference of a discrete Darboux transformation like we study here appeared in [22] in connection with the Toda lattice.

If $P = P_U P_L$ as in (2.2), then by reversing the order of multiplication we obtain another block tridiagonal matrix of the form

$$\widetilde{P} = P_L P_U = \begin{pmatrix} S_0 & 0 & \\ R_1 & S_1 & 0 \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} Y_0 & X_0 & \\ 0 & Y_1 & X_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} \widetilde{B}_0 & \widetilde{A}_0 & \\ \widetilde{C}_1 & \widetilde{B}_1 & \widetilde{A}_1 \\ & \ddots & \ddots & \ddots \end{pmatrix}. \tag{3.1}$$

Now the new block entries are given by (see (2.9) and (2.10))

$$\widetilde{A}_n = S_n X_n = \tau_n^{-1} \tau_{n+1}, \quad n \geq 0,$$
$$\widetilde{B}_n = R_n X_{n-1} + S_n Y_n = \tau_n^{-1}(\beta_n + \alpha_n)\tau_n = \tau_n^{-1}(\widehat{B}_n - \beta_{n+1} + \beta_n)\tau_n, \quad n \geq 0, \tag{3.2}$$
$$\widetilde{C}_n = R_n Y_{n-1} = \tau_n^{-1}(\beta_n \alpha_{n-1})\tau_{n-1} = \tau_n^{-1}(\beta_n \widehat{C}_{n-1} \beta_{n-1}^{-1})\tau_{n-1}, \quad n \geq 1.$$

The matrix $\widetilde{P}$ is actually stochastic, since the multiplication of two stochastic matrices is again a stochastic matrix. Therefore it is a new QBD process with block entries $\widetilde{A}_n$, $\widetilde{B}_n$ and $\widetilde{C}_n$. In fact we will get several QBD processes depending on many free parameters. In terms of a model driven by urn experiments (as we will see in Section 5) the factorization $P = P_U P_L$ may be thought as two urn experiments, Experiment 1 and Experiment 2, respectively. We first perform the Experiment 1 and with the result we immediately perform the Experiment 2. The urn model for $\widetilde{P} = P_L P_U$ will proceed in the reversed order, first the Experiment 2 and with the result the Experiment 1.

The same can be done for the LU factorization (2.5) of the form $P = \widetilde{P}_L \widetilde{P}_U$. The corresponding Darboux transformation is

$$\widehat{P} = \widetilde{P}_U \widetilde{P}_L = \begin{pmatrix} \widetilde{Y}_0 & \widetilde{X}_0 & \\ 0 & \widetilde{Y}_1 & \widetilde{X}_1 \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \widetilde{S}_0 & 0 & \\ \widetilde{R}_1 & \widetilde{S}_1 & 0 \\ & \ddots & \ddots & \ddots \end{pmatrix} = \begin{pmatrix} \widehat{B}_0 & \widehat{A}_0 & \\ \widehat{C}_1 & \widehat{B}_1 & \widehat{A}_1 \\ & \ddots & \ddots & \ddots \end{pmatrix}. \tag{3.3}$$

The new coefficients are given by (see (2.14))

$$\widehat{A}_n = \widetilde{X}_n \widetilde{S}_{n+1} = \widetilde{\tau}_n^{-1} \widetilde{\tau}_{n+1}, \quad n \geq 0,$$
$$\widehat{B}_n = \widetilde{X}_n \widetilde{R}_{n+1} + \widetilde{Y}_n \widetilde{S}_n = \widetilde{\tau}_n^{-1} (\widetilde{\beta}_{n+1} + \widetilde{\alpha}_n) \widetilde{\tau}_n, \quad n \geq 0,$$
$$\widehat{C}_n = \widetilde{Y}_n \widetilde{R}_n = \widetilde{\tau}_n^{-1} \widetilde{\alpha}_n \widetilde{\beta}_n \widetilde{\tau}_{n-1}, \quad n \geq 1.$$

If we assume that the block tridiagonal stochastic matrix P is self-adjoint (in some appropriate Hilbert space) then there exists a unique weight matrix W defined on the interval $-1 \leq x \leq 1$ (see [2,6]). Given such a weight matrix W we can consider the skew symmetric bilinear form defined for any pair of matrix-valued polynomials $P(x)$ and $Q(x)$ by the numerical matrix

$$(P,Q)_W := \int_{-1}^{1} P(x)W(x)Q^*(x)dx, \tag{3.4}$$

where $Q^*(x)$ denotes the conjugate transpose of $Q(x)$. This leads, using the Gram-Schmidt process, to the existence of a sequence of matrix-valued orthogonal polynomials Q_n with nonsingular leading coefficients satisfying a three-term recursion relation

$$xQ_n(x) = A_n Q_{n+1}(x) + B_n Q_n(x) + C_n Q_{n-1}(x), \quad n \geq 0, \tag{3.5}$$

where $Q_{-1}(x) = 0, Q_0(x) = I$ and A_n, B_n, C_n are the coefficients of the block tridiagonal matrix P. With all these ingredients we can get the corresponding Karlin-McGregor representation formula for the block entry (i,j) of P^n (see [2,6]). Indeed,

$$P_{ij}^n = (x^n Q_i, Q_j)_W (Q_j, Q_j)_W^{-1} = \left(\int_{-1}^{1} x^n Q_i(x)W(x)Q_j^*(x)dx \right) \left(\int_{-1}^{1} Q_j(x)W(x)Q_j^*(x)dx \right)^{-1}. \tag{3.6}$$

We can also compute the invariant measure $\boldsymbol{\pi}$ of the QBD process P in terms of the inverse of the norms $\Pi_n = (Q_n, Q_n)_W^{-1}$ (see Theorem 3.1 of [14]). Indeed, this invariant vector is given by

$$\boldsymbol{\pi} = \left((\Pi_0 \boldsymbol{e}_d)^T; (\Pi_1 \boldsymbol{e}_d)^T; (\Pi_2 \boldsymbol{e}_d)^T; \cdots \right), \tag{3.7}$$

where we recall here that $\boldsymbol{e}_d$ is the d-dimensional vector with all components equal to 1.

One important aspect of the Darboux transformation starting from the UL factorization is to study how to transform the *matrix-valued* spectral measure associated with a QBD process with one-step transition probability matrix P. The property of being self-adjoint may be lost for the Darboux transformation of P given by $\widetilde{P}$.

In the scalar case (tridiagonal matrix P) it is very well known that if the moment $\mu_{-1} = \int_{-1}^{1} d\omega(x)/x$ is well defined, where ω is the spectral measure associated with P, then a candidate for the family of spectral measures is then given by a *Geronimus transformation* of ω, i.e.

$$\widetilde{\omega}(x) = y_0 \frac{\omega(x)}{x} + M\delta_0(x), \quad M = 1 - y_0 \mu_{-1},$$

where $\delta_0(x)$ is the Dirac delta located at $x = 0$. Similarly, for the LU factorization, the corresponding Darboux transformation (3.3) $\widehat{P}$ gives rise a spectral measure $\widehat{\omega}$ given by a *Christoffel transformation* of ω, i.e. $\widehat{\omega}(x) = x\omega(x)$ (see [10] and references therein).

In the matrix-valued case it is possible to see (in analogy with the scalar case), that if the moment $\mu_{-1} = \int_{-1}^{1} dW(x)/x$ is well defined, then a candidate for the family of matrix-valued spectral measures associated with the Darboux transformation $\widetilde{P}$ is again a Geronimus transformation of W, i.e.

$$\widetilde{W}(x) = \frac{W(x)}{x} + \boldsymbol{M}\delta_0(x), \quad \boldsymbol{M} = \alpha_0^{-1}\mu_0 - \mu_{-1}, \tag{3.8}$$

as we will see in the example of the next section. Observe from the derivation of the coefficients $\widetilde{A}_n, \widetilde{B}_n, \widetilde{C}_n$ in (3.2), that the free parameters of $\widetilde{W}$ will only depend on α_0 and not on the sequence τ_n, which will only interfere in the normalization of the corresponding matrix-valued polynomials. In the case where α_0 is a singular matrix, we will have a degenerate matrix-valued spectral measure. Also we observe that $\widetilde{W}$ in general *is neither symmetric nor positive semidefinite*. In order for $\widetilde{W}$ to be a proper weight matrix, the matrix $\boldsymbol{M}$ in (3.8) has to be positive semidefinite.

Similarly, for the LU factorization, the corresponding Darboux transformation (3.3) $\widehat{P}$ gives rise to a block Jacobi matrix and a matrix-valued spectral measure $\widehat{W}$. It is possible to see that $\widehat{W}$ is given by a Christoffel transformation of W, i.e.

$$\widehat{W}(x) = xW(x).$$

In this case the weight matrix $\widehat{W}$ is unique and positive semidefinite.

4. The (Jacobi type) one-step example

In this section we will study a specific example coming from group representation theory, introduced for the first time in [12]. In [9] we studied the probabilistic aspects of this example and gave an explicit expression of the block entries A_n, B_n, C_n in (2.1). The most general situation is considered in [13], where the authors also give two stochastic models in terms of urns and Young diagrams.

First we will rewrite the block entries A_n, B_n, C_n introduced in [9] in a more convenient way (following the ideas of [13], see also [11]). For $\alpha, \beta > -1$ and $0 < k < \beta + 1$ define the coefficients

$$a_1(i,n) = \frac{(n+k)(n+\beta+d)}{(2n+\alpha+\beta+d+i)(n+k+d-i-1)}, \qquad b_1(i,n) = \frac{n(n+k+d-1)}{(2n+\alpha+\beta+d+i-1)(n+k+d-i-1)},$$

$$a_2(i,n) = \frac{(d-i-1)(\beta-k+i+1)}{(n+\alpha+\beta-k+2i+1)(n+k+d-i-1)}, \qquad b_2(i,n) = \frac{i(k+d-i-1)}{(n+\alpha+\beta-k+2i)(n+k+d-i-1)},$$

$$a_3(i,n) = \frac{(n+\alpha+i)(n+\alpha+\beta-k+d+i)}{(2n+\alpha+\beta+d+i)(n+\alpha+\beta-k+2i+1)}, \qquad b_3(i,n) = \frac{(n+\alpha+\beta+d+i-1)(n+\alpha+\beta-k+i)}{(2n+\alpha+\beta+d+i-1)(n+\alpha+\beta-k+2i)}.$$

Observe that all these coefficients are always *positive* for $i = 0, 1, \ldots, d-1$, $n \geq 0$, and that we have

$$a_1(i,n) + a_2(i,n) + a_3(i,n) = 1, \quad b_1(i,n) + b_2(i,n) + b_3(i,n) = 1. \tag{4.1}$$

Observe also that when $d \geq 2$ there is a new parameter k. The block entries A_n, B_n, C_n are given by

$$A_n = \sum_{i=0}^{d-1} a_1(i,n)b_3(i,n+1)E_{ii} + \sum_{i=0}^{d-2} a_1(i+1,n)b_2(i+1,n+1)E_{i+1,i},$$

$$B_n = \sum_{i=0}^{d-2} a_3(i+1,n)b_2(i+1,n)E_{i+1,i} + \sum_{i=0}^{d-2} a_2(i,n)b_3(i+1,n)E_{i,i+1}$$

$$+ \sum_{i=0}^{d-1} \left[a_1(i,n)b_1(i,n+1) + a_2(i,n)b_2(i+1,n) + a_3(i,n)b_3(i,n) \right] E_{ii},$$

$$C_n = \sum_{i=0}^{d-1} a_3(i,n)b_1(i,n)E_{ii} + \sum_{i=0}^{d-2} a_2(i,n)b_1(i+1,n)E_{i,i+1},$$

where E_{ij} denotes as usual the matrix with entry (i,j), which is equal to 1 and 0 elsewhere.

The family of matrix-valued polynomials generated by the three-term recursion relation (3.5), where $Q_{-1}(x) = 0$ and $Q_0(x) = I$, is in fact orthogonal with respect to the weight matrix (see [24] and [9])

$$W(x) = x^\alpha (1-x)^\beta V^* Z(x) V, \quad x \in [0,1], \tag{4.2}$$

where

$$Z(x) = \sum_{i,j=0}^{d-1} \left(\sum_{r=0}^{d-1} \binom{r}{i} \binom{r}{j} \binom{d+k-r-2}{d-r-1} \binom{\beta-k+r}{r} (1-x)^{i+j} x^{d-r-1} \right) E_{ij},$$

and V is the nonsingular upper triangular matrix

$$V = \sum_{i \leq j} (-1)^i \frac{(-j)_i}{(1-d)_i} \frac{(\alpha+\beta-k+j+1)_i}{(\beta-k+1)_i} E_{ij}.$$

Here $(a)_n = a(a+1)\cdots(a+n-1)$ denotes the Pochhammer symbol.

The way of writing the block entries A_n, B_n, C_n above is very useful when trying to find a particular factorization of the form $P = P_U P_L$ as in (2.2). Indeed, good candidates for the block entries X_n, Y_n, R_n, S_n are given by

$$X_n = \sum_{i=0}^{d-1} a_1(i,n) E_{ii}, \quad Y_n = \sum_{i=0}^{d-1} a_3(i,n) E_{ii} + \sum_{i=0}^{d-2} a_2(i,n) E_{i,i+1}, \tag{4.3}$$

$$R_n = \sum_{i=0}^{d-1} b_1(i,n) E_{ii}, \quad S_n = \sum_{i=0}^{d-1} b_3(i,n) E_{ii} + \sum_{i=0}^{d-2} b_2(i+1,n) E_{i+1,i}. \tag{4.4}$$

The relations (4.1) actually say that P_U and P_L are stochastic matrices. This factorization appeared for the first time in [13], but this *is not the only* UL stochastic factorization possible for the matrix P. As we saw in the previous section, the UL factorization comes with at least a free extra parameter α_0 which in this case is a $d \times d$ matrix with some restrictions.

We will see now how the choice of factors in [13] fits with the more general framework above, i.e. we give now a choice for α_0 and τ_n such that we get X_n, Y_n, R_n, S_n as in (4.3) and (4.4), i.e. as in [13].

Consider

$$\alpha_0 = B_0 - D_0, \tag{4.5}$$

where D_0 is the diagonal matrix

$$D_0 = \sum_{i=0}^{d-1} a_1(i,0) b_1(i,1) E_{ii} = \sum_{i=0}^{d-1} \frac{k(\beta+d)(k+d)}{(\alpha+\beta+d+i)_2 (k+d-i-1)_2} E_{ii}.$$

Observe that D_0 is the first summand in the diagonal entries of B_0. Let L_n be as in (2.6)[1] and choose

$$\tau_n = \tau_0 \left(L_n^{-1} \big|_{\alpha=\alpha-1} \right),$$

where τ_0 is a lower triangular matrix which inverse is given by the stochastic matrix

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[1] A different way of writing the lower triangular matrix L_n can be found in page 751 of [9] (written there as A_n^n).

$$\tau_0^{-1} = \sum_{i=0}^{d-1} \frac{\alpha+\beta-k+i}{\alpha+\beta-k+2i} E_{ii} + \sum_{i=0}^{d-2} \frac{i+1}{\alpha+\beta-k+2i+2} E_{i+1,i} = S_0.$$

Then the block entries X_n, Y_n, R_n, S_n in (2.10) coincide with the block entries X_n, Y_n, R_n, S_n given in [13] (see (4.3) and (4.4)). Moreover, the matrix-valued spectral measure $\widetilde{W}$ associated with the Darboux transformation $\widetilde{P} = P_L P_U$ (see (3.1)) is given by

$$\widetilde{W}(x) = \frac{W(x)}{x}, \quad x \in [0,1], \quad \alpha > 0, \quad \beta > -1, \quad 0 < k < \beta+1,$$

where W is the matrix-valued spectral measure associated with P (see (4.2)). Observe that α_0 in this case is chosen in such a way that $\boldsymbol{M} = \alpha_0^{-1}\mu_0 - \mu_{-1} = 0$ in (3.8), i.e. $\alpha_0 = \mu_0\mu_{-1}^{-1}$, an alternative to the expression for α_0 above.

If we consider the LU factorization of the same block tridiagonal P, let us choose

$$\widetilde{\tau}_n = \widetilde{\tau}_0 \left(L_n^{-1}\big|_{\alpha=\alpha+1} \right),$$

where $\widetilde{\tau}_0 = \tau_0^{-1}\big|_{\alpha=\alpha+1}$. Then the block entries $\widetilde{X}_n, \widetilde{Y}_n, \widetilde{R}_n, \widetilde{S}_n$ in (2.14) are given by

$$\widetilde{X}_n = X_n\big|_{\alpha=\alpha+1}, \quad \widetilde{Y}_n = Y_n\big|_{\alpha=\alpha+1}, \quad \widetilde{R}_n = R_n\big|_{\alpha=\alpha+1}, \quad \widetilde{S}_n = S_n\big|_{\alpha=\alpha+1}.$$

The matrix-valued spectral measure $\widehat{W}$ associated with the Darboux transformation $\widehat{P} = \widetilde{P}_U \widetilde{P}_L$ of P (see (3.3)) is given by the Christoffel transformation of W, i.e.

$$\widehat{W}(x) = xW(x), \quad x \in [0,1], \quad \alpha, \beta > -1, \quad 0 < k < \beta+1.$$

As we said earlier, the choice of α_0 above is the one that among the possible factorizations of P reproduces the results in [13].

Let us focus now in the case where α_0 is not necessarily chosen as in (4.5). For simplicity, we will explore only the case where $d = 2$. The case $d = 1$ was already studied in [10], along with an urn model for the Jacobi polynomials (for a different urn model for the Jacobi polynomials which does not exploit the factorization of the tridiagonal matrix see [7]).

4.1. Case $d = 2$

The coefficients of P given earlier become now

$$A_n = \begin{pmatrix} \frac{(\beta+n+2)(k+n)(\alpha+\beta+n+2)}{(k+n+1)(\alpha+\beta+2n+2)(\alpha+\beta+2n+3)} & 0 \\ \frac{k(\beta+n+2)}{(\alpha+\beta-k+n+3)(\alpha+\beta+2n+3)(k+n+1)} & \frac{(\beta+n+2)(\alpha+\beta+n+3)(\alpha+\beta-k+n+2)}{(\alpha+\beta+2n+3)(\alpha+\beta+2n+4)(\alpha+\beta-k+n+3)} \end{pmatrix}, \tag{4.6}$$

$$B_n = \begin{pmatrix} B_n^{11} & \frac{(\beta-k+1)(\alpha+\beta+n+2)}{(k+n+1)(\alpha+\beta+2n+2)(\alpha+\beta-k+n+2)} \\ \frac{(\alpha+n+1)k}{(k+n)(\alpha+\beta-k+n+2)(\alpha+\beta+2n+3)} & B_n^{22} \end{pmatrix}, \tag{4.7}$$

$$C_n = \begin{pmatrix} \frac{n(\alpha+n)(\alpha+\beta-k+n+2)}{(\alpha+\beta-k+n+1)(\alpha+\beta+2n+1)(\alpha+\beta+2n+2)} & \frac{n(\beta-k+1)}{(\alpha+\beta-k+n+1)(\alpha+\beta+2n+2)(k+n)} \\ 0 & \frac{n(\alpha+n+1)(k+n+1)}{(k+n)(\alpha+\beta+2n+2)(\alpha+\beta+2n+3)} \end{pmatrix}, \tag{4.8}$$

where

$$B_n^{11} = \frac{(n+k)(n+\beta+2)(n+1)}{(\alpha+\beta+2n+2)(n+k+1)(\alpha+\beta+2n+3)}$$
$$+ \frac{(n+\alpha)(\alpha+\beta-k+n+2)(n+\alpha+\beta+1)}{(\alpha+\beta+2n+2)(\alpha+1+n-k+\beta)(\alpha+\beta+2n+1)}$$
$$+ \frac{k(\beta-k+1)}{(\alpha+1+n-k+\beta)(n+k+1)(\alpha+\beta-k+n+2)(n+k)},$$

and

$$B_n^{22} = \frac{(n+\beta+2)(n+1)(n+k+2)}{(\alpha+\beta+2n+3)(\alpha+\beta+2n+4)(n+k+1)}$$
$$+ \frac{(\alpha+n+1)(\alpha+\beta+n+2)(\alpha+1+n-k+\beta)}{(\alpha+\beta+2n+3)(\alpha+\beta+2n+2)(\alpha+\beta-k+n+2)}.$$

The main difference with the scalar case ($d = 1$) is that we have a new parameter $0 < k < \beta + 1$. A straightforward computation, using the definition of $a_j(i,n), b_j(i,n), j = 1,2,3$, gives

$$L_n = \begin{pmatrix} \frac{(n+k)(\alpha+\beta+n+2)_n}{k(\beta+2)_n} & 0 \\ -\frac{n(\alpha+\beta+n+3)_n}{(\alpha+\beta-k+2)(\beta+2)_n} & \frac{(\alpha+\beta+n-k+2)(\alpha+\beta+n+3)_n}{(\alpha+\beta-k+2)(\beta+2)_n} \end{pmatrix}.$$

The coefficients α_n, β_n of the UL factorization (2.8) are going to be computed by using the expressions (2.9). Since the matrix α_0 is in principle any 2×2 matrix, the coefficients α_n, β_n are not easy to find. Once we have these coefficients we can compute τ_n by solving (2.12) and (2.13), which now also may yield more degrees of freedom.

We first review in this $d = 2$ case what we did earlier for general d.

If we choose α_0 as in (4.5), i.e.

$$\alpha_0 = \begin{pmatrix} \frac{\beta-k+1}{(1+\alpha+\beta-k)(1+k)(2+\alpha+\beta-k)} + \frac{\alpha(2+\alpha+\beta-k)}{(2+\alpha+\beta)(1+\alpha+\beta-k)} & \frac{\beta-k+1}{(1+k)(2+\alpha+\beta-k)} \\ \frac{1+\alpha}{(3+\alpha+\beta)(2+\alpha+\beta-k)} & \frac{(1+\alpha)(1+\alpha+\beta-k)}{(3+\alpha+\beta)(2+\alpha+\beta-k)} \end{pmatrix}, \tag{4.9}$$

then the explicit expression for τ_n is given by

$$\tau_0^{-1}\tau_n = \begin{pmatrix} \frac{k(\beta+2)_n}{(n+k)(\alpha+\beta+n+1)_n} & 0 \\ \frac{n(\beta+2)_n}{(n+k)(\alpha+\beta+n-k+1)(\alpha+\beta+n+1)_n} & \frac{(\alpha+\beta-k+1)(\beta+2)_n}{(\alpha+\beta+n-k+1)(\alpha+\beta+n+2)_n} \end{pmatrix} = \left(L_n^{-1} \big|_{\alpha=\alpha-1} \right),$$

where

$$\tau_0^{-1} = \begin{pmatrix} 1 & 0 \\ \frac{1}{\alpha+\beta-k+2} & \frac{\alpha+\beta-k+1}{\alpha+\beta-k+2} \end{pmatrix}. \tag{4.10}$$

The block entries of the stochastic matrices P_U and P_L are given by

$$X_n = \begin{pmatrix} \frac{(n+k)(n+\beta+2)}{(2n+\alpha+\beta+2)(n+k+1)} & 0 \\ 0 & \frac{n+\beta+2}{2n+\alpha+\beta+3} \end{pmatrix}, \quad Y_n = \begin{pmatrix} \frac{(n+\alpha)(n+\alpha+\beta-k+2)}{(2n+\alpha+\beta+2)(n+\alpha+1-k+\beta)} & \frac{\beta-k+1}{(n+\alpha+1-k+\beta)(n+k+1)} \\ 0 & \frac{n+\alpha+1}{2n+\alpha+\beta+3} \end{pmatrix},$$
$$\tag{4.11}$$

$$S_n = \begin{pmatrix} \frac{n+\alpha+\beta+1}{2n+\alpha+\beta+1} & 0 \\ \frac{k}{(n+\alpha+\beta-k+2)(n+k)} & \frac{(n+\alpha+\beta+2)(n+\alpha+1-k+\beta)}{(2n+\alpha+\beta+2)(n+\alpha+\beta-k+2)} \end{pmatrix}, \quad R_n = \begin{pmatrix} \frac{n}{2n+\alpha+\beta+1} & 0 \\ 0 & \frac{n(n+k+1)}{(2n+\alpha+\beta+2)(n+k)} \end{pmatrix}. \tag{4.12}$$

We will give in the next section an interpretation of these matrices in terms of an urn model.

We are done with trying to reproduce the results in [13] and we move on to a generic α_0 where things are more complicated. The only thing that we know is that α_0 must be at least semi-stochastic (see Remark 2.1).

Getting away from (4.9), let us put

$$\alpha_0 = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}.$$

According to (3.8), the family of matrix-valued spectral measures associated with the Darboux transformation $\widetilde{P}$ is given by

$$\widetilde{W}(x) = \frac{W(x)}{x} + \boldsymbol{M}\delta_0(x), \quad \boldsymbol{M} = \alpha_0^{-1}\mu_0 - \mu_{-1}. \tag{4.13}$$

In the case of this example we have that

$$\mu_0 = \frac{\Gamma(\alpha+1)\Gamma(\beta+2)(\alpha+\beta-k+2)}{\Gamma(\alpha+\beta+3)}\begin{pmatrix} 1 & 0 \\ 0 & \frac{(\alpha+1)(k+1)}{(\alpha+\beta+3)(\beta-k+1)} \end{pmatrix},$$

and (assuming $\alpha > 0, \beta > -1$)

$$\mu_{-1} = \frac{\Gamma(\alpha)\Gamma(\beta+2)}{\Gamma(\alpha+\beta+2)}\begin{pmatrix} \alpha+\beta-k+1 & -1 \\ -1 & \frac{(\alpha+1)(k+1)(\alpha+\beta-k+2)-k(\beta-k+1)}{(\alpha+\beta+2)(\beta-k+1)} \end{pmatrix}.$$

Observe that we have the following relation between the moments μ_0 and μ_{-1}:

$$\mu_0|_{\alpha=\alpha-1} = \tau_0^{-1}\mu_{-1}\tau_0^{-*},$$

where τ_0^{-1} is the lower triangular matrix (4.10). As we mentioned in Section 3, $\widetilde{W}$ is in general neither symmetric nor positive semidefinite. It is easy to see that $\boldsymbol{M}$ in (4.13) is symmetric if and only if one of the entries of α_0 is chosen according to the following relation

$$s_{12} = \frac{(\beta-k+1)(\alpha+\beta+3)}{(\alpha+1)(k+1)}s_{21}. \tag{4.14}$$

In what follows we will study two special cases where we can explicitly analyze the different values of the parameters s_{ij} for which the Darboux transformation gives rise to a QBD process. In the first case we will focus on the positivity of the matrix-valued spectral measure $\widetilde{W}$ in (4.13), while in the second case we will analyze the stochastic block factorization without looking at the positivity or the symmetry of $\widetilde{W}$.

(1) Let us choose for convenience

$$\alpha_0 = \begin{pmatrix} \frac{(\alpha+\beta+3)(\beta-k+1)}{(k+1)(\alpha+1)(\alpha+\beta-k+1)}s_{11} & \frac{(\alpha+\beta+3)(\beta-k+1)}{(k+1)(\alpha+1)}s_{21} \\ s_{21} & (\alpha+\beta-k+1)s_{21} \end{pmatrix}, \tag{4.15}$$

where s_{11} and s_{21} are in principle free parameters. Since condition (4.14) is satisfied, $\widetilde{W}$ in (4.13) is a symmetric matrix. The determinant of α_0 is given by

$$|\alpha_0| = \frac{(\alpha+\beta+3)(\beta-k+1)}{(k+1)(\alpha+1)}s_{21}(s_{11}-s_{21}).$$

A straightforward computation shows that $\boldsymbol{M}$ can be written in this case as

$$\boldsymbol{M} = \tau_0 \begin{pmatrix} \frac{(\alpha)_2(k+1)(\alpha+\beta-k+2)}{(\beta-k+1)(\alpha+\beta+2)_2(s_{11}-s_{21})} - 1 & 0 \\ 0 & \frac{\alpha+1}{(\alpha+\beta+2)(\alpha+\beta-k+2)s_{21}} - 1 \end{pmatrix} \mu_0|_{\alpha=\alpha-1} \tau_0^*,$$

where τ_0 is the inverse of the lower triangular matrix (4.10). Since μ_0 is diagonal, then $\boldsymbol{M}$ is positive semidefinite if the parameters s_{11} and s_{21} are chosen in the following range

$$0 < s_{21} \leq \frac{\alpha+1}{(\alpha+\beta+3)(\alpha+\beta-k+2)}, \tag{4.16}$$

$$s_{21} < s_{11} \leq s_{21} + \frac{(\alpha)_2(k+1)(\alpha+\beta-k+2)}{(\beta-k+1)(\alpha+\beta+2)_2}.$$

Based on what happens in the scalar case, one could expect that if we choose s_{11} and s_{21} in the range above, then we should get a stochastic block factorization of P of the form (2.2), where P_U and P_L are also stochastic matrices. However, *this is not true*. In fact the condition on the positivity of the entries of X_n, Y_n, S_n, R_n will force us to modify the upper bound of the second inequality in (4.16).

Another important point is the choice of the sequence of matrices τ_n such that (2.12) and (2.13) hold and the entries of the matrices X_n, Y_n, S_n, R_n in (2.10) are all nonnegative. Since τ_n is a 2×2 matrix, it has 4 degrees of freedom for every n. For simplicity, we look for *lower triangular matrices* τ_n with 3 degrees of freedom for every n. The diagonal entries of τ_n can be given by solving the equations (2.12) and (2.13). Then, the matrices X_n and S_n are always lower triangular, while the matrices Y_n and R_n are both full matrices. In order to surmise the remaining free parameter of τ_n, we force Y_n to be upper triangular and as a consequence R_n will be also upper triangular. These conditions will give us explicitly τ_n for every n and one sees that the sum of every row of P_U and P_L is always 1.

Finally, we need all entries of X_n, Y_n, S_n, R_n to be nonnegative. The entries of these matrices are rational functions depending on s_{11} and s_{21}. After extensive symbolic computations we find that all entries of X_n, Y_n, S_n, R_n are nonnegative (and therefore P_U and P_L are stochastic matrices) if the parameters s_{11} and s_{21} are chosen in the following range

$$0 < s_{21} \leq \frac{\alpha+1}{(\alpha+\beta+3)(\alpha+\beta-k+2)},$$

$$s_{21} < s_{11} \leq \frac{s_{21}\left(s_{21} - \frac{(\alpha+1)^2(k+1)}{k(\beta-k+1)(\alpha+\beta+3)}\right)}{s_{21} - \frac{(\alpha+1)(k+1)}{k(\alpha+\beta-k+1)(\alpha+\beta+3)}}.$$

Observe that the singular point of the rational function of s_{21} above is to the right of the upper bound of s_{21} in (4.16). In Fig. 1 we can see this region for the special values of $\alpha = 3, \beta = 2, k = 1$. The green line (above the shaded area of the figure) is the upper bound for which $\boldsymbol{M}$ is positive semidefinite, but we observe here that there may be values of s_{11}, s_{21} for which $\boldsymbol{M}$ is positive semidefinite, and yet the block entries X_n, Y_n, S_n, R_n do not have all their entries nonnegative.

This concludes our look at the case when α_0 was chosen as in (4.15).

(2) Let us focus now exclusively on the block entries X_n, Y_n, S_n, R_n and the sequence of matrices τ_n chosen to guarantee that P_U and P_L are stochastic without looking into the matrix-valued spectral measure $\widetilde{W}$ resulting after the Darboux transformation. It was mentioned in the previous case that we can always choose a unique sequence of lower triangular matrices τ_n such that (2.12) and (2.13) hold and X_n and S_n are lower triangular matrices while Y_n and R_n are upper triangular matrices. Imagine now that we would like to have one (or several) of the matrices X_n, Y_n, S_n, R_n as a *diagonal one*. To insure this we need to impose some restrictions on the parameters s_{ij} of α_0. There are four possible situations:
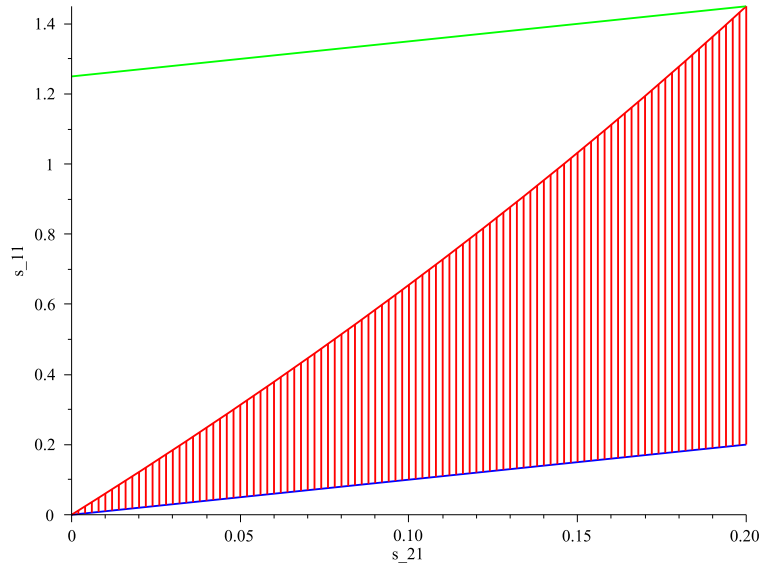
Fig. 1. The region with red stripes (shaded area) gives all possible values of s_{21} and s_{11} for which all entries of X_n, Y_n, S_n, R_n are nonnegative for the values of $\alpha = 3, \beta = 2, k = 1$. The green line (above the shaded area) is the upper bound for which M is positive semidefinite. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

(a) X_n *diagonal*: the matrix α_0 should be chosen as the two-parameter family of matrices

$$\alpha_0 = \begin{pmatrix} s_{11} & s_{12} \\ \frac{1+\alpha}{(3+\alpha+\beta)(2+\alpha+\beta-k)} & \frac{(1+\alpha)(1+\alpha+\beta-k)}{(3+\alpha+\beta)(2+\alpha+\beta-k)} \end{pmatrix}.$$

Observe that the second row is the same as the second row of α_0 in (4.9).

(b) R_n *diagonal*: the matrix α_0 should be chosen as the two-parameter family of matrices

$$\alpha_0 = \begin{pmatrix} s_{11} & \frac{\beta-k+1}{(1+k)(2+\alpha+\beta-k)} \\ s_{21} & \frac{(1+\alpha)(1+\alpha+\beta-k)}{(3+\alpha+\beta)(2+\alpha+\beta-k)} \end{pmatrix}.$$

Observe that the second column is the same as the second column of α_0 in (4.9).

(c) Y_n *diagonal*: the matrix α_0 should be chosen as the two-parameter family of singular matrices

$$\alpha_0 = \begin{pmatrix} 0 & 0 \\ s_{21} & s_{22} \end{pmatrix}.$$

(d) S_n *diagonal*: the matrix α_0 should be chosen as the two-parameter family of singular matrices

$$\alpha_0 = \begin{pmatrix} 0 & s_{21} \\ 0 & s_{22} \end{pmatrix}.$$

Let us analyze further the case (a) (the rest can be studied in a similar manner). For convenience we will work with the normalization

$$\alpha_0 = \begin{pmatrix} \left[\frac{\beta-k+1}{(1+\alpha+\beta-k)(1+k)(2+\alpha+\beta-k)} + \frac{\alpha(2+\alpha+\beta-k)}{(2+\alpha+\beta)(1+\alpha+\beta-k)} \right] s_{11} & \frac{\beta-k+1}{(1+k)(2+\alpha+\beta-k)} s_{12} \\ \frac{1+\alpha}{(3+\alpha+\beta)(2+\alpha+\beta-k)} & \frac{(1+\alpha)(1+\alpha+\beta-k)}{(3+\alpha+\beta)(2+\alpha+\beta-k)} \end{pmatrix}.$$

Then, all entries of X_n, Y_n, S_n, R_n are nonnegative (and therefore P_U and P_L are stochastic matrices) if s_{11} and s_{12} are chosen in the following range
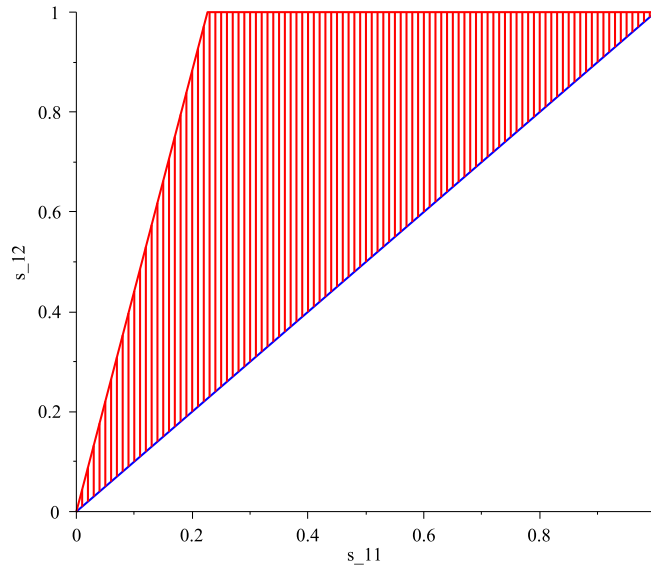
Fig. 2. The region with red stripes (shaded area) gives all possible values of s_{11} and s_{12} for which all entries of X_n, Y_n, S_n, R_n are nonnegative for the values of $\alpha = 1, \beta = 2, k = 2$.

$$0 < s_{11} \leq 1,$$

$$s_{11} \leq s_{12} \leq \min\left\{\left(1 + \frac{\alpha(k+1)(\alpha + \beta - k + 2)^2}{(\alpha + \beta + 2)(\beta - k + 1)}\right) s_{11}, 1\right\}.$$

In Fig. 2 we can visualize this region for the special values of $\alpha = 1, \beta = 2, k = 2$. Since in general the condition (4.14) is not satisfied, then there is no symmetric and positive definite spectral measure $\widetilde{W}$ of the form (4.13) for the Darboux transformation $\widetilde{P}$. Nevertheless, if we consider the monic matrix-valued polynomials $\widetilde{P}_n$ generated by the Jacobi matrix $\widetilde{J} = \boldsymbol{\beta\alpha}$ (see (2.8)), then they are *left-orthogonal* (i.e. $(\widetilde{P}_n, \widetilde{P}_m)_{\widetilde{W}} = 0$ for $n > m$, see (3.4)) with respect to the matrix-valued function (4.13), with

$$\boldsymbol{M} = \tau_0 \begin{pmatrix} \frac{(\alpha)_2}{(\alpha+\beta+2)_2 |\alpha_0|} - 1 & \frac{(\beta-k+1)(\alpha+1)(1-s_{12})}{|\alpha_0|(k+1)(\alpha+\beta+3)(\alpha+\beta-k+2)} \\ 0 & 0 \end{pmatrix} \mu_0|_{\alpha=\alpha-1} \, \tau_0^*,$$

where τ_0 is the inverse of the lower triangular matrix (4.10). Observe that $\boldsymbol{M}$ is a singular and non-symmetric matrix. Observe also that the only case where $\boldsymbol{M}$ is symmetric is given by choosing $s_{12} = 1$. But this is just the first case obtained by taking

$$s_{21} = \frac{\alpha + 1}{(\alpha + \beta + 2)(\alpha + \beta - k + 2)}.$$

Remark 4.1. We would like to remark on a special property of the matrix-valued orthogonal polynomials $\widetilde{P}_n$ generated by the Darboux transformation of P for the case $s_{12} = 1$ above. It is well known that the original matrix-valued orthogonal polynomials P_n satisfy a second-order differential equation of the form

$$P_n''(x)F_2(x) + P_n'(x)F_1(x) + P_n(x)F_0 = \Lambda_n P_n(x), \tag{4.17}$$

where $F_2(x) = x(1-x)I$ and F_1, F_0 certain matrix polynomials of degree 1 and 0, respectively (see for instance [24] or [9]). In this situation (and only in this situation) the matrix-valued polynomials $\widetilde{P}_n$ obtained by performing the Darboux transformation also satisfy a *second-order differential equation* of the form (4.17) with coefficients $\widetilde{F}_2, \widetilde{F}_1, \widetilde{F}_0$ given by

$$\widetilde{F}_2(x) = x\left[\begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix}x + \begin{pmatrix} \frac{\beta-k+1}{\alpha+\beta-k+2} & -\frac{\beta-k+1}{\alpha+\beta-k+2} \\ -\frac{\alpha+1}{\alpha+\beta-k+2} & \frac{\alpha+1}{\alpha+\beta-k+2} \end{pmatrix}\right],$$

$$\widetilde{F}_1(x) = x\begin{pmatrix} 0 & 0 \\ k+1 & -(\alpha+\beta+3) \end{pmatrix} + \begin{pmatrix} -\frac{\beta-k+1}{\alpha+\beta-k+2} & -\frac{(\beta-k+1)(\alpha+\beta-k+1)}{\alpha+\beta-k+2} \\ \frac{\alpha+1}{\alpha+\beta-k+2} & \frac{(\alpha+1)(\alpha+\beta-k+1)}{\alpha+\beta-k+2} \end{pmatrix},$$

$$\widetilde{F}_0 = \begin{pmatrix} (k+1)(\alpha+\beta-k+1) & 0 \\ -(k+1) & 0 \end{pmatrix}.$$

Typically, in the scalar case, and for some special values of the parameters involved, the order of the differential equation satisfied by the new polynomials after a Darboux transformation is higher than 2. The remarkable fact in the matrix case is that we have a family of matrix-valued orthogonal polynomials $\widetilde{P}_n$ (depending on one free parameter s_{11}) satisfying *the same second-order* differential equation with coefficients *independent* of s_{11}. This phenomenon is not new and appeared for the first time in [3] using a method different than the Darboux transformation. For other examples of the bispectral property following a Darboux transformation see [8].

Remark 4.2. Once we have the explicit expression of the matrix-valued spectral measure W associated with P (or $\widetilde{W}$ associated with $\widetilde{P}$, or $\widehat{W}$ associated with $\widehat{P}$) we can use the Karlin-McGregor representation formula (3.6) to get the n-step transition probability matrix P^n by computing the first matrix-valued orthogonal polynomials Q_n. We can also compute the invariant measure $\boldsymbol{\pi}$ for the process P using formula (3.7). An invariant measure for the process P at hand was computed in [9]. Finally we can also study recurrence associated with the process P. According to Theorem 8.1 of [9], the QBD process that results from P is never positive recurrent. If $-1 < \beta \leq 0$, then the process is null recurrent. If $\beta > 0$, then the process is transient. Therefore recurrence is independent of the value of α. The QBD processes $\widetilde{P}$ and $\widehat{P}$ will inherit the same recurrence behavior as the original P, since the matrix-valued spectral measures $\widetilde{W}$ and $\widehat{W}$ will have the same behavior as W at $x = 1$ (see [9] for details).

We hope that the discussion above gives an indication of the many possibilities that open up in the matrix-valued case. A relatively simple instance is discussed in the next section.

## 5. An urn model for the 2×2 matrix-valued orthogonal polynomials

We now give an urn model associated with the 2×2 matrix-valued orthogonal polynomials of Jacobi type given in the previous section. For this purpose we will focus on the simplest case of the UL block factorization $P = P_U P_L$ with block entries X_n, Y_n, S_n, R_n given by (4.11) and (4.12). In [13] one finds another urn model associated with this example, but different from the one to be given here.

From now on, it will be assumed that the parameters α, β and k are nonnegative integers with $1 \leq k \leq \beta$. Consider the discrete-time QBD process on $\mathbb{Z}_{\geq 0} \times \{1, 2\}$ whose one-step transition probability matrix P is given by the coefficients A_n, B_n and C_n in (4.6), (4.7) and (4.8), respectively. Consider the UL factorization $P = P_U P_L$ (2.2) with coefficients X_n, Y_n, S_n, R_n given by (4.11) and (4.12). Each one of these matrices P_U and P_L will give rise to an experiment in terms of an urn model, which we call Experiment 1 and Experiment 2, respectively. For simplicity, we will consider these two experiments as discrete-time Markov chains on $\mathbb{Z}_{\geq 0}$ with transitions between not only adjacent states but second adjacent ones too. At times $t = 0, 1, 2, \ldots$ an urn A contains n blue balls and this determines the state of our Markov chain on $\mathbb{Z}_{\geq 0}$ at that time. All the urns we use in both experiments sit in a bath consisting of an infinite number of blue and red balls.

Experiment 1 (for P_U) will give a discrete-time pure-birth QBD process on $\mathbb{Z}_{\geq 0} \times \{1, 2\}$ with diagram given by
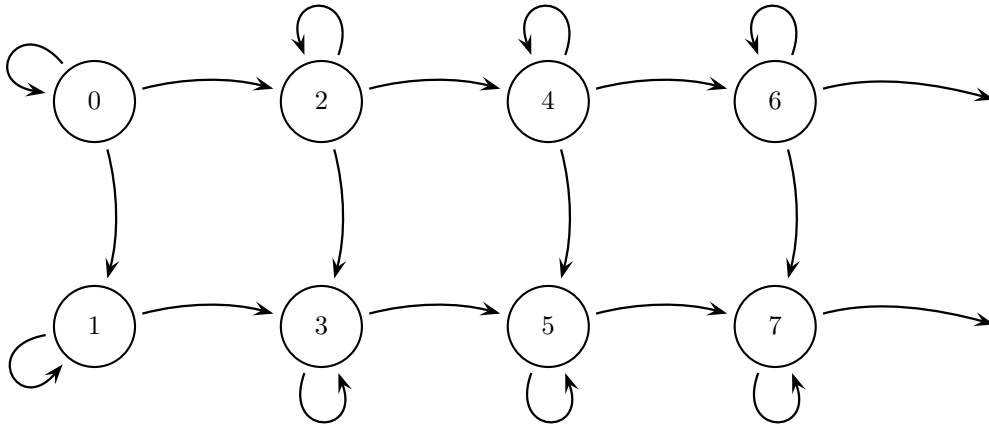
This latter diagram can also be viewed as a pure-birth discrete-time Markov chain on $\mathbb{Z}_{\geq 0}$ with transitions between not only adjacent states but second adjacent ones too. Let us call this chain $\{Z_t^{(1)} : t = 0, 1, \ldots\}$. A diagram of the same situation is now given by
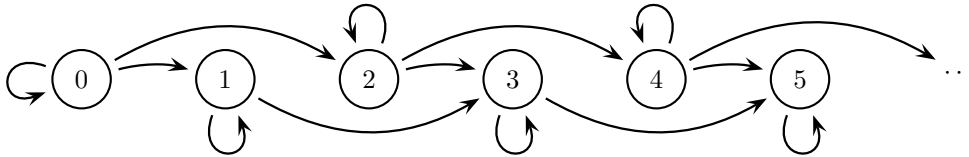
We will construct an urn model for this last diagram. Assume the urn A contains n blue balls ($n \geq 0$) at time 0 (i.e. $Z_0^{(1)} = n$). The transition mechanism will depend on the parity of n.

Consider first the case where n is odd and write $n = 2m + 1, m \geq 0$. Remove $m + 1$ blue balls from the urn A until we have m blue balls. Take $\beta + 2$ blue balls and $m + \alpha + 1$ red balls from the bath and add them to the urn. Draw one ball from the urn at random with the uniform distribution. We have two possibilities:

- If we get a blue ball then we remove/add balls until we have $2m + 3$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(1)} = n + 2 \,|\, Z_0^{(1)} = n, \; n = 2m + 1\right) = \frac{m + \beta + 2}{2m + \alpha + \beta + 3}.$$

  Observe that this probability is given by entry $(2, 2)$ of X_m in (4.11).
- If we get a red ball then we remove/add balls until we have $2m + 1$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(1)} = n \,|\, Z_0^{(1)} = n, \; n = 2m + 1\right) = \frac{m + \alpha + 1}{2m + \alpha + \beta + 3}.$$

  Observe that this probability is given by entry $(2, 2)$ of Y_m in (4.11).

Consider now the case where n is even and write $n = 2m, m \geq 0$. Again, remove m blue balls from the urn A until we have m blue balls. Additionally we will have two other urns, one painted in blue, which we call B, and the other one painted in red, which we call R. These urns are initially empty and will be emptied after their use in going from one time step to the next.

In urn A we add α blue balls and $\beta - k + 1$ red balls. In urn B we place $m + \alpha + \beta - k + 2$ blue balls and $m + k$ red balls. In urn R we place $m + k$ blue balls and 1 red ball. These balls are taken from the bath.

Draw one ball from urn A at random with the uniform distribution. If we get a blue ball then we go to the urn B and draw a ball, while if we get a red ball then we go the urn R and draw a ball. We have three possibilities:

- If we get two blue balls in a row, i.e. one from urn A and then one from urn B, then we remove/add balls until we have $2m$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(1)} = n \,|\, Z_0^{(1)} = n, \ n = 2m\right) = \frac{(m+\alpha)(m+\alpha+\beta-k+2)}{(2m+\alpha+\beta+2)(m+\alpha+1-k+\beta)}.$$

Observe that this probability is given by entry $(1,1)$ of Y_m in (4.11).

- If we get two red balls in a row, i.e. one from urn A and then one from urn R, then we remove/add balls until we have $2m+1$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(1)} = n+1 \,|\, Z_0^{(1)} = n, \ n = 2m\right) = \frac{\beta-k+1}{(m+\alpha+\beta-k+1)(m+k+1)}.$$

Observe that this probability is given by entry $(1,2)$ of Y_m in (4.11).

- If we get either a blue and a red ball or a red and a blue ball then we remove/add balls until we have $2m+2$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(1)} = n+2 \,|\, Z_0^{(1)} = n, \ n = 2m\right) = \frac{(m+k)(m+\beta+2)}{(2m+\alpha+\beta+2)(m+k+1)}.$$

Observe that this probability is given by entry $(1,1)$ of X_m in (4.11).

We are done describing Experiment 1 and we move on to describe an unrelated experiment.

Experiment 2 (for P_L) will give a discrete-time pure-death QBD process on $\mathbb{Z}_{\geq 0} \times \{1,2\}$ with diagram given by
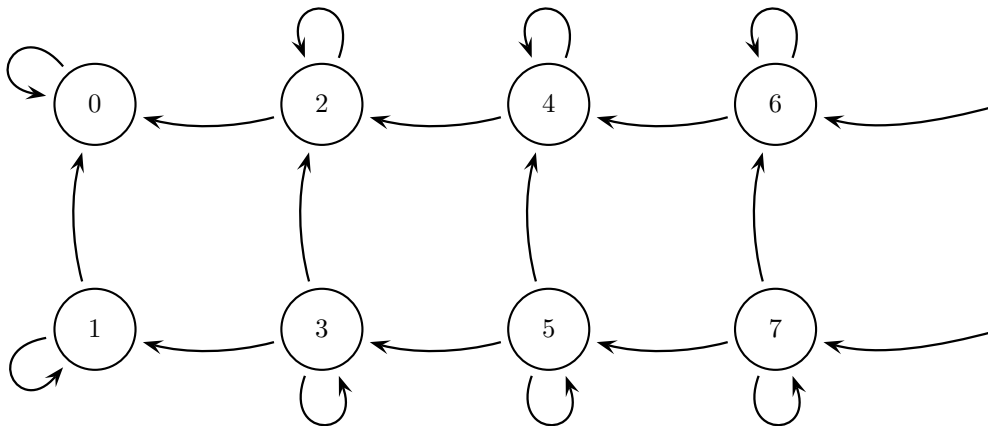
Again, this last diagram can also be viewed as a pure-death discrete-time Markov chain on $\mathbb{Z}_{\geq 0}$ with transitions between not only adjacent states but second adjacent ones too, and with an absorbing state at 0. Let us call this chain $\{Z_t^{(2)} : t = 0, 1, \ldots\}$. A diagram of the same situation is now given by
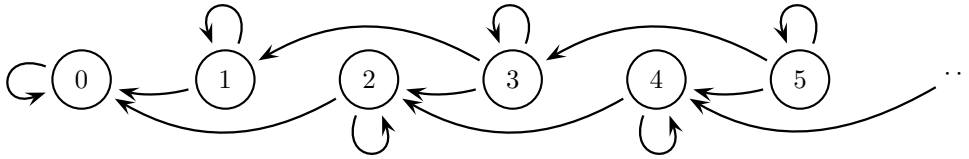
We will construct an urn model for this last diagram. Assume that urn A contains n blue balls ($n \geq 1$) at time 0 (i.e. $Z_0^{(0)} = n$). The state $n = 0$ is absorbing. Consider first the case where n is even and write $n = 2m, m \geq 1$. Remove m blue balls from the urn A until we have m blue balls. Take $m + \alpha + \beta + 1$ red balls from the bath and add them to the urn. Draw one ball from the urn at random with the uniform distribution. We have two possibilities:

- If we get a blue ball then we remove/add balls until we have $2m - 2$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(2)} = n - 2 \,|\, Z_0^{(2)} = n, \ n = 2m\right) = \frac{m}{2m + \alpha + \beta + 1}.$$

  Observe that this probability is given by entry $(1,1)$ of R_m in (4.12).
- If we get a red ball then we remove/add balls until we have $2m$ blue balls at the urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(2)} = n \,|\, Z_0^{(2)} = n, \ n = 2m\right) = \frac{m + \alpha + \beta + 1}{2m + \alpha + \beta + 1}.$$

  Observe that this probability is given by entry $(1,1)$ of S_m in (4.12).

Consider now the case where n is odd and write $n = 2m + 1, m \geq 0$. Again, remove $m + 1$ blue balls from the urn A until we have m blue balls. Additionally we will have two other urns, one painted in blue, which we call B, and the other one painted in red, which we call R. Again, these urns are initially empty and will be emptied after their use in going from one time step to the next.

In urn A we add $m + \alpha + \beta - k + 1$ blue balls and 1 red ball. In urn B we place $m + \alpha + \beta + 2$ blue balls and m red balls. In urn R we place m blue balls and k red balls. Draw one ball from urn A at random with the uniform distribution. If we get a blue ball then we go to the urn B and draw a ball, while if we get a red ball then we go the urn R and draw a ball. We have three possibilities:

- If we get two blue balls in a row, i.e. one from urn A and then one from urn B, then we remove/add balls until we have $2m + 1$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(2)} = n \,|\, Z_0^{(2)} = n, \ n = 2m + 1\right) = \frac{(m + \alpha + \beta + 2)(m + \alpha + 1 - k + \beta)}{(2m + \alpha + \beta + 2)(m + \alpha + \beta - k + 2)}.$$

  Observe that this probability is given by entry $(2,2)$ of S_m in (4.12).
- If we get two red balls in a row, i.e. one from urn A and then one from urn R, then we remove/add balls until we have $2m$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(2)} = n - 1 \,|\, Z_0^{(2)} = n, \ n = 2m + 1\right) = \frac{k}{(m + \alpha + \beta - k + 2)(m + k)}.$$

  Observe that this probability is given by entry $(2,1)$ of S_m in (4.12).
- If we get either a blue and a red ball or a red and a blue ball then we remove/add balls until we have $2m - 1$ blue balls in urn A and start over. Therefore

$$\mathbb{P}\left(Z_1^{(2)} = n - 2 \mid Z_0^{(2)} = n, \ n = 2m + 1\right) = \frac{m(m + k + 1)}{(2m + \alpha + \beta + 2)(m + k)}.$$

Observe that this probability is given by entry $(2, 2)$ of R_m in (4.12).

The urn model for P (on $\mathbb{Z}_{\geq 0}$) will be the composition of Experiment 1 and then Experiment 2, while the urn model for the Darboux transformation $\widetilde{P}$ (3.1) proceeds in the reversed order. Observe from Remark 4.2 and since α, β and k are nonnegative integers with $1 \leq k \leq \beta$ that this urn model will always be transient. Similar urn models can be derived for the LU factorization with small modifications.

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