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Multivariate Krawtchouk Polynomials and Composition Birth and Death Processes

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Abstract: This paper defines the multivariate Krawtchouk polynomials, orthogonal on the multinomial distribution, and summarizes their properties as a review. The multivariate Krawtchouk polynomials are symmetric functions of orthogonal sets of functions defined on each of N multinomial trials. The dual multivariate Krawtchouk polynomials, which also have a polynomial structure, are seen to occur naturally as spectral orthogonal polynomials in a Karlin and McGregor spectral representation of transition functions in a composition birth and death process. In this Markov composition process in continuous time, there are N independent and identically distributed birth and death processes each with support $0, 1, \dots$. The state space in the composition process is the number of processes in the different states $0, 1, \dots$. Dealing with the spectral representation requires new extensions of the multivariate Krawtchouk polynomials to orthogonal polynomials on a multinomial distribution with a countable infinity of states.

Keywords: Bernoulli trials and orthogonal polynomials; birth and death processes; composition Markov processes; Karlin and McGregor spectral representation; multivariate Krawtchouk polynomials

MSC: 33D52; 60J27

1. Introduction

Griffiths [1] and Diaconis and Griffiths [2] construct multivariate Krawtchouk polynomials orthogonal on the multinomial distribution and study their properties. Recent representations and derivations of the orthogonality of these polynomials are in [3–6].

The authors emphasise different approaches to the multivariate orthogonal polynomials. The approach of Diaconis and Griffiths [2] is probabilistic and directed to Markov chain applications; the approach of Iliev [5] is via Lie groups; and the physics approach of Genest *et al.* [3] is as matrix elements of group representations on oscillator states. Xu [7] studies discrete multivariate orthogonal polynomials, which have a triangular construction of products of one-dimensional orthogonal polynomials. They are particular cases of the polynomials in this paper; see Diaconis and Griffiths [2]. These polynomials extend the Krawtchouk polynomials on the binomial distribution to a general class of multi-dimensional orthogonal polynomials on the multinomial distribution. They appear naturally in composition Markov chains as eigenfunctions in a diagonal expansion of the transition functions. There are many interesting examples of these Markov chains in Zhou and Lange [8]. Binomial and multinomial random variables can be constructed as a sum of independent and identically distributed random variables, which are indicator functions of the events that occur on each of N trials. The Krawtchouk and multivariate Krawtchouk polynomials are symmetric functions of orthogonal functions sets on each of the trials. The simplest case is the Krawtchouk polynomials where the representation is explained in Section 2. In the multivariate Krawtchouk polynomials, there is not a unique orthogonal function set on trials with multiple outcomes greater than two, so the polynomials depend on which orthogonal function set is taken for a basis on the trials.

A well-known spectral expansion by Karlin and McGregor [9–11] for the transition functions $\{p_{ij}(t)\}_{i,j=0}^{\infty}$ of a birth and death process with rates $\lambda_i, \mu_i, i = 0, 1, \dots$ is that:

$$p_{ij}(t) = \pi_j \int_0^{\infty} e^{-zt} Q_i(z) Q_j(z) \psi(dz), \quad i, j = 0, 1, \dots \quad (1)$$

where $\{Q_i\}_{i=1}^{\infty}$ are orthogonal polynomials on the spectral measure ψ , which is a probability measure, and:

$$\pi_j = \frac{\lambda_0 \cdots \lambda_{j-1}}{\mu_1 \cdots \mu_j}, \quad j = 1, 2, \dots \quad (2)$$

A number of classical birth and death processes have a spectral expansion where the orthogonal polynomials are constructed from the Meixner class. This class has a generating function of the form:

$$G(v, z) = h(v) e^{xu(v)} = \sum_{m=0}^{\infty} Q_m(z) v^m / m! \quad (3)$$

where $h(v)$ is a power series in t with $h(0) = 1$ and $u(v)$ is a power series with $u(0) = 0$ and $u'(0) \neq 0$. Meixner [12] characterizes the class of weight functions and orthogonal polynomials with the generating function Equation (3). They include the Krawtchouk polynomials, Poisson–Charlier polynomials, scaled Meixner polynomials and Laguerre polynomials (the Meixner orthogonal polynomials are a specific set belonging to the Meixner class with a name in common). A general reference to these orthogonal polynomials is Ismail [13].

In this paper, the spectral expansion is extended to composition birth and death processes, where there are N independent and identically distributed birth and death processes operating and $\{X(t)\}_{t \geq 0}$ is such that the i -th element $\{X_i(t)\}_{t \geq 0}$ counts the number of processes in state i at time t . In the analogue of Equation (1), the spectral polynomials are the dual multivariate Krawtchouk polynomials. The dual polynomial system is therefore very important, and attention is paid to describing it.

There are extensions of the multivariate Krawtchouk polynomials to multivariate orthogonal polynomials on the multivariate Meixner distribution and multivariate product Poisson distribution, where they occur as eigenfunctions of multi-type birth and death processes [14].

This paper defines the multivariate Krawtchouk polynomials, summarizes their properties, then considers how they are found in spectral expansions of composition birth and death processes. It is partly a review of these polynomials and is self-contained. For a fuller treatment, see Diaconis and Griffiths [15]. The polynomials are naturally defined by a generating function, and so, generating function techniques are used extensively in the paper. Probabilistic notation is used, particularly the expectation operator \mathbb{E} , which is a linear operator acting on functions of random variables, which take discrete values in this paper. If X_1, \dots, X_d are random variables, then:

$$\mathbb{E}[f(X_1, \dots, X_d)] = \sum_{x_1, \dots, x_d} f(x_1, \dots, x_d) P(X_1 = x_1, \dots, X_d = x_d) \quad (4)$$

Often, orthogonal polynomials are regarded as random variables. For example, $\{K_n(X; N, p)\}_{n=0}^N$ are the one-dimensional Krawtchouk polynomials as random variables and:

$$\begin{aligned} \mathbb{E}[K_n(X; N, p) K_m(X; N, p)] &= \sum_{x=0}^N K_n(x; N, p) K_m(x; N, p) \binom{N}{x} p^x q^{N-x} \\ &= \delta_{mn} n!^2 \binom{N}{n} (pq)^n, \quad m, n = 0, 1, \dots, N \end{aligned} \quad (5)$$

where $q = 1 - p$. A convention of using capital letters for random variables and lower case for values that they take is used, except when the random variables are denoted by Greek letters, when they have to be considered in context.

Section 2, Theorem 1, shows how the Krawtchouk polynomials can be expressed as elementary symmetric functions of N Bernoulli trials, centred at their mean p . The Meixner orthogonal polynomials on the geometric distribution are also expressed as functions of an infinity of centred Bernoulli trials in Theorem 2. There is some, but not total symmetry in this expression. Krawtchouk polynomials occur naturally as eigenfunctions in Ehrenfest urn processes, and the eigenfunction expansion of their transition functions is explained in Section 2.3. Section 3 introduces the multivariate Krawtchouk polynomials, explaining how they are constructed in a symmetric way from a product set of orthogonal functions on N independent multinomial trials. The dual orthogonal system is described and a scaling found, so that they are multivariate Krawtchouk polynomials on a different multinomial distribution in Theorem 3. The polynomial structure of the multivariate Krawtchouk polynomials is described in Theorem 4 and the structure in the dual system in Theorem 5. Recurrence relationships are found for the system in Theorem 6 and for the dual system in Theorem 7. The dual recurrence relationship is used to identify the polynomials as eigenfunctions in a d -type Ehrenfest urn in Theorem 8. In Section 3.2, a new extension is made to multivariate Krawtchouk polynomials where there are an infinite number of possibilities in each multinomial trial. These polynomials occur naturally as eigenfunctions in composition birth and death processes in a Karlin and McGregor spectral expansion in Theorem 9. Theorem 10 considers the polynomial structure of the dual polynomials in the spectral expansion. Theorem 11 gives an interesting identity for these spectral polynomials in composition birth and death processes when the spectral polynomials in the individual processes belong to the Meixner class.

2. Bernoulli Trials and Orthogonal Polynomials

The paper begins with expressing the one-dimensional Krawtchouk polynomials as symmetric functions of Bernoulli trials. The multivariate Krawtchouk polynomials are extensions of this construction in higher dimensions.

2.1. Krawtchouk Orthogonal Polynomials

The Krawtchouk orthogonal polynomials $\{K_n(x; N, p)\}_{n=0}^N$ are orthogonal on the binomial (N, p) distribution:

$$\binom{N}{x} p^x q^{N-x}, \quad x = 0, 1, \dots, N \quad (6)$$

They have a generating function:

$$G(z; x) = \sum_{n=0}^N K_n(x; N, p) \frac{z^n}{n!} = (1 + qz)^x (1 - pz)^{N-x} \quad (7)$$

The scaling is such that the polynomials $K_n(x; N, p)/n!$ are monic and:

$$\begin{aligned} \mathbb{E}[K_n(X; N, p)^2] &= \sum_{x=0}^N \binom{N}{x} p^x q^{N-x} K_n(x; N, p)^2 \\ &= n!^2 \binom{N}{n} (pq)^n \end{aligned} \quad (8)$$

If the Krawtchouk polynomials are scaled to be $Q_n(x)$, so that $Q_n(0) = 1$, then there is a duality that $Q_n(x) = Q_x(n)$. A binomial random variable X counts the number of successes in N independent trials, each with a probability p of success. Let $\zeta_i = 1$ if the i -th trial is a success and $\zeta_i = 0$ otherwise. Then, $\{\zeta_i\}_{i=1}^N$ is a sequence of Bernoulli trials with $P(\zeta_i = 1) = p$, $P(\zeta_i = 0) = q$, and $X = \sum_{i=1}^N \zeta_i$. It is interesting to express the Krawtchouk polynomials as symmetric functions of $\{\zeta_i\}_{i=1}^N$. If there is just one trial with $N = 1$, $X = \zeta_1$, and the orthogonal polynomial set on X is $\{1, \zeta_1 - p\}$. There can only be a constant function and a linear function if there are just two values that ζ_1 can take. A product set of

orthogonal functions on $\{\xi_i\}_{i=1}^N$ is $\otimes_{i=1}^N \{1, \xi_i - p\}$, and we want to form a smaller basis from these functions to orthogonal polynomials in $X = \sum_{i=1}^N \xi_i$.

Theorem 1. The Krawtchouk polynomials are proportional to the elementary symmetric functions of $\{\xi_i - p\}_{i=1}^N$;

$$K_n(X; N, p) = n! \sum_{\sigma \in S_N} (\xi_{\sigma(1)} - p) \cdots (\xi_{\sigma(n)} - p) \tag{9}$$

where S_N is the symmetric group on $\{1, 2, \dots, N\}$.

Proof. A generating function for the symmetric functions on the right of Equation (9) is:

$$\sum_{n=0}^N \frac{z^n}{n!} n! \sum_{\sigma \in S_N} (\xi_{\sigma(1)} - p) \cdots (\xi_{\sigma(n)} - p) = \prod_{i=1}^N (1 + z(\xi_i - p)) \tag{10}$$

If x of the ξ_i are one and $N - x$ are zero, then Equation (10) is equal to:

$$(1 + z(1 - p))^X (1 - zp)^{N-X} \tag{11}$$

identical to the right side of Equation (7). Therefore, Equation (9) holds since the generating functions of both sides, regarding X as a random variable, are the same. \square

The representation Equation (9) of the Krawtchouk polynomials appears with a full treatment in Diaconis and Griffiths [15] and very briefly as the generating function proof above in Griffiths [1]. The author is not aware of any other appearances of Equation (9).

2.2. Meixner Polynomials on the Geometric Distribution

The Meixner orthogonal polynomials on the geometric distribution are orthogonal on:

$$pq^x, \quad x = 0, 1, \dots \tag{12}$$

Let $\{\xi_i\}_{i=1}^\infty$ be a sequence of Bernoulli trials. Let X count the number of trials $\xi_i = 0$ before the first trial where $\xi_{x+1} = 1$. That is $X = \sum_{j=1}^\infty \prod_{i=1}^{j-1} (1 - \xi_i) \xi_j$. X is clearly not a symmetric function of $\{\xi_i\}_{i=1}^\infty$. The orthogonal polynomials on the geometric distribution are a special case of the general Meixner polynomials and have a generating function:

$$G(z; x) = \sum_{n=0}^\infty M_n(x; 1, q) z^n = (1 - q^{-1}z)^x (1 - z)^{-(x+1)} \tag{13}$$

A product set of orthogonal functions on the trials is:

$$\bigotimes_{i=1}^\infty \{1, \xi_i - p\} \tag{14}$$

It is of interest to express the orthogonal polynomial set $\{M_n(x; 1, q)\}_{n=0}^\infty$ as a series expansion in the product set Equation (14) as a comparison of what happens with the Krawtchouk polynomials. A calculation is now made of $\mathbb{E}[(\xi_{i_1} - p) \cdots (\xi_{i_r} - p) G(z; X)]$ leading to coefficients in the expansion of the Meixner polynomials in the product set of orthogonal functions. Given $X = x$, it must be that $\xi_j = 0, j = 1, \dots, x, \xi_{x+1} = 1$ and $\{\xi_j\}_{j=x+2}^\infty$ are distributed as Bernoulli trials. Therefore:

$$\mathbb{E}[(\xi_{i_1} - p) \cdots (\xi_{i_r} - p) | X = x] = \begin{cases} 0 & \text{if } i_r \geq x + 2, \\ q(-p)^{r-1} & \text{if } i_r = x + 1, \\ (-p)^r & \text{if } i_r \leq x. \end{cases} \tag{15}$$

Taking an expectation conditional on X , then over X ,

$$\begin{aligned} &\mathbb{E}[(\xi_{i_1} - p) \cdots (\xi_{i_r} - p)G(z; X)] \\ &= q(-p)^{r-1}G(z; i_r - 1)pq^{i_r-1} + \sum_{j=i_r}^{\infty} (-p)^r G(z; j)pq^j \\ &= (-1)^{r-1}p^r q^{i_r} z G(z; i_r - 1) \end{aligned} \tag{16}$$

Simplification to the last line is straightforward, so it is omitted. Considering the coefficients of z^n in Equation (16) and using Theorem 1 gives the following theorem.

Theorem 2. Let $\{\xi_i\}_{i=1}^{\infty}$ be a sequence of Bernoulli (p) trials and $X = \sum_{j=1}^{\infty} \prod_{i=1}^{j-1} (1 - \xi_i)\xi_j$. Then, X has a geometric distribution, and the Meixner polynomials on this geometric distribution have a representation for $n \geq 1$ of:

$$\begin{aligned} M_n(X; 1, q) &= \sum_{r=1}^{\infty} \sum_{i_1 < \cdots < i_r} (\xi_{i_1} - p) \cdots (\xi_{i_r} - p) (-1)^{r-1} q^{i_r-r} M_{n-1}(i_r - 1; 1, q) \\ &= \sum_{r=1}^{\infty} \sum_{l=r}^{\infty} \frac{1}{(r-1)!} K_{r-1}(X_l; l, p) (\xi_l - p) (-1)^{r-1} q^{l-r} M_{n-1}(l-1; 1, q) \end{aligned} \tag{17}$$

where $X_l = \xi_1 + \cdots + \xi_l$.

2.3. An Ehrenfest urn

The Krawtchouk polynomials appear naturally as eigenfunctions in an Ehrenfest urn model. This is explored in Diaconis and Griffiths [15]. An urn has N balls coloured red or blue. Transitions occur at rate one when a ball is chosen at random, and the colour of the ball is changed according to a transition matrix:

$$P = \begin{bmatrix} 0 & 1 \\ q/p & 1 - q/p \end{bmatrix} \tag{18}$$

where $p, q > 0$, $p + q = 1$ and $q \leq p$. Let $\{X(t)\}_{t \geq 0}$ be the number of red balls in the urn at time t . That is, if a blue ball is chosen, it is changed to red with probability one, whereas if a red ball is chosen, it is changed to blue with probability q/p . $\{X(t)\}_{t \geq 0}$ is a reversible Markov process, which is a birth and death process, with a Binomial (N, p) stationary distribution.

The process is a composition Markov process in the following sense. Label the balls $1, 2, \dots, N$ at time $t = 0$ and keep the labels over time as their colours change. Let $\{\xi_i(t)\}_{t \geq 0}$ describe the colour of ball i at time t : $\xi_i(t) = 1$ if the i -th ball is red or zero if the ball is blue. The processes $\{\xi_i(t)\}_{t \geq 0}$, $i = 1, \dots, N$ are independent; each has a rate of events $1/N$ when the specified ball is chosen; and $X(t) = \sum_{i=1}^N \xi_i(t)$. Denote $p_{ij}(t) = P(\xi_k(t) = j \mid \xi_k(0) = i)$, for $i, j = 1, 2$. Standard Markov process theory gives that:

$$P(t) = \begin{bmatrix} q + pe^{-\lambda t} & p(1 - e^{-\lambda t}) \\ q(1 - e^{-\lambda t}) & p + qe^{-\lambda t} \end{bmatrix} \tag{19}$$

where $\lambda = 1/(Np)$. It is immediate that the stationary distribution of each of the labelled processes is (p, q) . An eigenvalue-eigenfunction expansion of $P(t)$ is:

$$P_{\eta, \xi}(t) = \pi_{\xi} \{1 + e^{-\lambda t} (pq)^{-1} (\eta - p) (\xi - p)\}, \xi, \eta = 0, 1 \tag{20}$$

where π_{ξ} is the stationary distribution with $\pi_0 = q$, $\pi_1 = p$. It is straightforward to check the agreement with $P(t)$ by substituting the four values of $\eta, \xi = 0, 1$.

In the Ehrenfest urn composition process, the transitions are made from $X(0) = x$ to $X(t) = y$ if $\sum_{i=1}^N \eta_i = x$ and $\sum_{i=1}^N \xi_i = y$. The transition probabilities are:

$$\begin{aligned}
 P(X(t) = y \mid X(0) = x) &= \sum_{\sigma \in S_N} P_{\eta_1 \xi_{\sigma(1)}}(t) \cdots P_{\eta_N \xi_{\sigma(N)}}(t) \\
 &= \binom{N}{y} p^y (1-p)^{N-y} \left\{ 1 + \sum_{n=1}^N e^{-\lambda n t} (pq)^{-n} \binom{N}{n}^{-1} \right. \\
 &\quad \times \left. \sum_{\sigma \in S_N} (\eta_{\sigma(1)} - p) \cdots (\eta_{\sigma(n)} - p) \sum_{\tau \in S_N} (\xi_{\tau(1)} - p) \cdots (\xi_{\tau(n)} - p) \right\} \\
 &= \binom{N}{y} p^y (1-p)^{N-y} \\
 &\quad \times \left\{ 1 + \sum_{n=1}^N e^{-\lambda n t} (pq)^{-n} (n!)^{-2} \binom{N}{n}^{-1} K_n(x; N, p) K_n(y; N, p) \right\} \tag{21}
 \end{aligned}$$

The Krawtchouk polynomials thus appear naturally as elementary symmetric functions of the individual labelled indicator functions in the Markov process.

3. Multivariate Krawtchouk Polynomials

The multivariate Krawtchouk polynomials with elementary basis \mathbf{u} were first constructed by Griffiths [1]. A recent introduction to them is Diaconis and Griffiths [2]. They play an important role in the spectral expansion of transition functions of composition Markov processes. Zhou and Lange [8], Khare and Zhou [16] have many interesting examples of such Markov processes. Later in this paper, we consider the particular composition processes where there are N particles independently performing birth and death processes.

The multivariate Krawtchouk polynomials are orthogonal on the multinomial distribution:

$$m(\mathbf{x}; \mathbf{p}) = \binom{N}{\mathbf{x}} \prod_{j=1}^d p_j^{x_j}, \quad x_j \geq 0, \quad j = 1, \dots, d, \quad |\mathbf{x}| = N \tag{22}$$

with $\mathbf{p} = \{p_j\}_{j=1}^d$ a probability distribution. Let J_1, \dots, J_N be independent and identically distributed random variables specifying outcomes on the N trials, such that:

$$P(J = k) = p_k, \quad k = 1, \dots, d \tag{23}$$

Then:

$$X_i = |\{J_k : J_k = i, k = 1, \dots, N\}| \tag{24}$$

Let $\mathbf{u} = \{u^{(l)}\}_{l=0}^{d-1}$ be an orthogonal set of functions on $\mathbf{p} = \{p_k\}_{k=1}^d$ with $u^{(0)} = 1$ satisfying:

$$\sum_{i=1}^d u_i^{(l)} u_i^{(m)} p_i = a_l \delta_{lm}, \quad l, m = 0, \dots, d-1 \tag{25}$$

This notation for the orthogonal set of functions follows Lancaster [17]. There is an equivalence that:

$$h_{il} = u_i^{(l-1)} \sqrt{p_i / a_{l-1}}, \quad i, l = 1, \dots, d \tag{26}$$

are elements of a $d \times d$ orthogonal matrix H . In this paper, $\{u^{(l)}\}_{l=0}^{d-1}$ are usually orthonormal functions with $a_l = 1, l = 0, 1, \dots, d-1$, unless stated otherwise. The one-dimensional Krawtchouk polynomials are constructed from a symmetrized product set of orthogonal functions $\otimes \{1, \xi_i - p\}_{i=1}^N$, and the construction of the multivariate polynomials follows a similar, but more complicated procedure.

Instead of having two unique elements in each orthogonal function set, there is a choice of orthogonal basis, and the construction is from the product set $\otimes_{i=1}^N \{u_{j_i}^{(l_i)}\}_{l_i=0}^{d-1}$. The orthogonality Equation (25) is equivalent to:

$$\mathbb{E}[u_{j_k}^{(l)} u_{j_k}^{(m)}] = a_l \delta_{lm} \tag{27}$$

for $k = 1, \dots, N$. Define a collection of orthogonal polynomials $\{Q_n(\mathbf{X}; \mathbf{u})\}$ with $\mathbf{n} = (n_1, \dots, n_{d-1})$ and $|\mathbf{n}| \leq N$ on the multinomial distribution as symmetrized elements from the product set, such that the sum is over products $u_{j_1}^{(l_1)} \dots u_{j_N}^{(l_N)}$ with $n_k = |\{l_i : l_i = k, k = 1, \dots, N\}|$ for $k = 1, \dots, d - 1$. $Q_n(\mathbf{X}; \mathbf{u})$ is the coefficient of $w_1^{n_1} \dots w_{d-1}^{n_{d-1}}$ in the generating function:

$$\begin{aligned} G(\mathbf{x}, \mathbf{w}, \mathbf{u}) &= \prod_{i=1}^N \left(1 + \sum_{l_i=1}^{d-1} w_{l_i} u_{j_i}^{(l_i)}\right) \\ &= \prod_{j=1}^d \left(1 + \sum_{l=1}^{d-1} w_l u_j^{(l)}\right)^{x_j} \end{aligned} \tag{28}$$

In the one-dimensional case $u_1^{(1)} = 0 - p_1 = -p_1, u_2^{(1)} = 1 - p_1$, orthogonal on $1 - p_1, p_1$, so the generating function is:

$$(1 - p_1 w_1)^{x_1} (1 + (1 - p_1) w_1)^{x_2} \tag{29}$$

which is, of course, the generating function of the Krawtchouk polynomials. x_1, x_2 are respectively the number of zero and one values in the N trials. It is straightforward to show, by using the generating function Equation (28), that:

$$\begin{aligned} \mathbb{E}[Q_m(\mathbf{X}; \mathbf{u}) Q_n(\mathbf{X}; \mathbf{u})] &= \sum_{\{\mathbf{x} : |\mathbf{x}|=N\}} Q_m(\mathbf{x}; \mathbf{u}) Q_n(\mathbf{x}; \mathbf{u}) m(\mathbf{x}; \mathbf{p}) \\ &= \delta_{mn} \binom{N}{\mathbf{n}^+} \prod_{j=1}^{d-1} a_j^{n_j} \end{aligned} \tag{30}$$

where $\mathbf{n}^+ = (n_0, \dots, n_{d-1})$, with $n_0 = N - \sum_{j=1}^{d-1} n_j$. Instead of indexing the polynomials by $\mathbf{n} = (n_1, \dots, n_{d-1})$, they could be indexed by \mathbf{n}^+ . This notation is sometimes convenient to use in the paper. The dual orthogonality relationship is, immediately from Equation (30),

$$\sum_{\{\mathbf{n} : |\mathbf{n}| \leq N\}} \binom{N}{\mathbf{n}^+}^{-1} \prod_{j=1}^{d-1} a_j^{-n_j} Q_n(\mathbf{x}; \mathbf{u}) Q_n(\mathbf{y}; \mathbf{u}) = \delta_{xy} m(\mathbf{x}, \mathbf{p})^{-1} \tag{31}$$

Expanding the generating function Equation (28) shows that:

$$Q_n(\mathbf{X}; \mathbf{u}) = \sum_{\{r : r_k = n_k\}} \frac{\prod_{j=1}^d x_j^{r_{[j]}}!}{\prod_{j=1}^d \prod_{k=1}^{d-1} r_{jk}!} \prod_{j=1}^d \prod_{k=1}^{d-1} \left(u_j^{(k)}\right)^{r_{jk}} \tag{32}$$

where \cdot indicates summation over an index and $a_{[b]} = a(a - 1) \dots (a - b + 1)$ for non-negative integers b . The dual generating function is:

$$\begin{aligned} &\sum_{\{\mathbf{x} : |\mathbf{x}|=N\}} \binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} v_1^{x_1} \dots v_d^{x_d} Q_n(\mathbf{x}; \mathbf{u}) \\ &= \left(\sum_{j=1}^d v_j\right)^{n_0} \prod_{i=1}^{d-1} \left(\sum_{j=1}^d v_j u_j^{(i)}\right)^{n_i} \end{aligned} \tag{33}$$

Expanding the generating function:

$$\binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} Q_n(\mathbf{x}; \mathbf{u}) = \sum_{\{r_i: r_i = n_i, r_j = x_j\}} \frac{\prod_{i=0}^{d-1} n_i!}{\prod_{i=0}^{d-1} \prod_{j=1}^d r_{ij}!} \prod_{i=1}^{d-1} \prod_{j=1}^d (u_j^{(i)})^{r_{ij}} \tag{34}$$

The two generating function Equations (28) and (33) are similar, and there is a form of self-duality for the polynomials. Let:

$$\omega_i^{(j)} = u_{j+1}^{(i-1)}, j = 0, \dots, d - 1, i = 1, \dots, d \tag{35}$$

Then, because of Equation (25):

$$\sum_{l=1}^d \omega_l^{(i)} \omega_l^{(k)} a_{l-1}^{-1} = \delta_{ik} p_i^{-1} \tag{36}$$

The right side of Equation (33) is equal to:

$$\prod_{i=1}^d \left(\sum_{j=0}^{d-1} \omega_i^{(j)} v_{j+1} \right)^{n_{i-1}} \tag{37}$$

which, apart from the different indexing and non-constant function $\omega^{(0)}$, generates multivariate Krawtchouk polynomials. Suppose that $\omega_i^{(0)} \neq 0$ for $i = 1, \dots, d$. Scale by letting $\hat{\omega}_i^{(j)} = \omega_i^{(j)} / \omega_i^{(0)}$, so that $\hat{\omega}_i^{(0)} = 1$. The orthogonality of these functions is:

$$\sum_{l=1}^d \hat{\omega}_l^{(i)} \hat{\omega}_l^{(j)} a_{l-1}^{-1} \omega_l^{(0)2} = \delta_{ij} p_i^{-1} \tag{38}$$

Let $\mathbf{b} = \{b_l\}_{l=1}^d$ be the scaled probability distribution of $\{a_{l-1}^{-1} \omega_l^{(0)2}\}_{l=1}^d$, so:

$$\sum_{l=1}^d \hat{\omega}_l^{(i)} \hat{\omega}_l^{(j)} b_l = \delta_{ij} \left(p_i \sum_{l=1}^d a_{l-1}^{-1} \omega_l^{(0)2} \right)^{-1} \tag{39}$$

The following theorem is evident from Equations (33) and (37), once the indexing is sorted out.

Theorem 3. There is a duality

$$\binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} Q_n(\mathbf{x}; \mathbf{u}) = \prod_{i=1}^d (\omega_i^{(0)})^{n_{i-1}} Q_{\mathbf{x}^-}^*(\mathbf{n}^+; \hat{\omega}) \tag{40}$$

where $Q_{\mathbf{x}^-}^*(\mathbf{n}^+; \hat{\omega})$, with $\mathbf{x}^- = (x_2, \dots, x_d)$, $\sum_{j=2}^d x_j \leq N$, are multivariate Krawtchouk polynomials, orthogonal on $m(\mathbf{n}^+; \mathbf{b})$.

There is an interesting identity when \mathbf{u} is self-dual with an indexing of j beginning from zero instead of one. That is:

$$u_j^{(l)} = u_l^{(j)}, j, l = 0, 1, \dots, n \tag{41}$$

Then indexing $\mathbf{x} = (x_0, \dots, x_n)$,

$$\binom{N}{\mathbf{n}^+}^{-1} Q_n(\mathbf{x}; \mathbf{u}) = \binom{N}{\mathbf{x}}^{-1} Q_{\mathbf{x}}(\mathbf{n}^+; \mathbf{u}^*) \tag{42}$$

where $u_j^{(l)*} = u_l^{(j)}$. This duality occurs in the scaled Krawtchouk polynomial basis, orthogonal on a binomial (n, p) distribution.

The emphasis in Theorem 3 is on considering the dual system, obtaining $\hat{\omega}$ from \mathbf{u} ; however, sometimes, it is natural to construct \mathbf{u} from an orthogonal set $\hat{\omega}$, particularly when $\omega_i^{(0)} = 1, i = 1, \dots, d$ and $\hat{\omega} = \omega$. Then, the polynomials on the left of Equation (40) are defined by the dual polynomials on the right. Later in the paper, it will be seen that this is natural in composition birth and death Markov processes.

The polynomial structure of the multivariate Krawtchouk polynomials is detailed in the next theorem.

Theorem 4. Define $U_l = \sum_{k=1}^N u_{jk}^{(l)} = \sum_{j=1}^d u_j^{(l)} X_j$ for $l = 1, \dots, d - 1$. $Q_n(\mathbf{X}; \mathbf{u})$ is a polynomial of degree $|\mathbf{n}|$ in (U_1, \dots, U_{d-1}) whose only term of maximal degree $|\mathbf{n}|$ is $\prod_{k=1}^{d-1} U_k^{n_k}$.

Proof. A method of proof is to consider the transform of $Q_n(\mathbf{X}; \mathbf{u})$, which is given by:

$$E \left[\prod_{j=1}^d \phi_j^{X_j} Q_n(\mathbf{X}; \mathbf{u}) \right] = \binom{N}{|\mathbf{n}|} \binom{|\mathbf{n}|}{\mathbf{n}} T_0(\phi)^{N-|\mathbf{n}|} T_1(\phi)^{n_1} \dots T_{d-1}(\phi)^{n_{d-1}} \tag{43}$$

where:

$$T_i(\phi) = \sum_{j=1}^d p_j \phi_j u_j^{(i)}, \quad i = 0, \dots, d - 1 \tag{44}$$

This transform is easily found by taking the transform of the generating function Equation (28). One can see directly that $Q_n(\mathbf{X}; \mathbf{u})$ is an orthogonal polynomial by considering the transform:

$$E \left(\prod_{j=1}^d X_{j[k_j]} \phi_j^{X_j} \right) = N_{[k]} \prod_{j=1}^d (\phi_j p_j)^{k_j} \cdot \left(\sum_{i=1}^d p_i \phi_i \right)^{N-|k|} \tag{45}$$

From Equations (43) and (45), $Q_n(x)$ is a polynomial of degree $|\mathbf{n}|$, whose only leading term is:

$$\frac{\prod_{i=1}^{d-1} S_i^{n_i}}{\prod_{i=1}^{d-1} n_i!} \tag{46}$$

This is seen by noting that the leading term is found by replacing $\phi_j p_j$ by X_j in:

$$N_{[|\mathbf{n}|]}^{-1} \binom{N}{|\mathbf{n}|} \binom{|\mathbf{n}|}{\mathbf{n}} T_1(\phi)^{n_1} \dots T_{d-1}(\phi)^{n_{d-1}} \tag{47}$$

Since we can replace $X_{j[k_j]}$ by X^{k_j} in considering the leading term of Equation (43) and setting $\phi_i = 1$ for $i = 1, \dots, d$. \square

The next theorem explains the polynomial structure in the dual system.

Theorem 5. Let $\{u^{(j)}\}_{j=0}^d$ be such that $u_1^{(j)} = 1$ for $j = 0, \dots, d - 1$, as well as the usual assumption that $u_i^{(0)} = 1$ for $i = 1, \dots, d$. Define $\kappa_l = \sum_{j=0}^{d-1} u_l^{(j)} n_j, l = 2, \dots, d$. Then, $\binom{N}{\mathbf{n}+}^{-1} Q_n(\mathbf{x}; \mathbf{u})$ is a polynomial of total degree $\sum_{i=2}^d x_i$ in $\{\kappa_l\}_{l=2}^d$ whose only term of maximal degree is $\prod_{l=2}^d \kappa_l^{x_l}$.

Proof. This follows from Theorem 3, with $\omega_i^{(0)} = 1, i = 1, \dots, d$, and Theorem 4. \square

There are recurrence relationships for the multivariate Krawtchouk polynomials, which are found here from a generating function approach; for another different proof, see Theorem 6.1 in Iliev [5]. Note that his multivariate Krawtchouk polynomials are scaled differently as

$$Q_n(\mathbf{x}; \mathbf{u}) \binom{N}{\mathbf{n}+}^{-1} \tag{48}$$

In Theorems 6–8, \mathbf{u} is taken to be orthonormal on \mathbf{p} , so $a_l = 1, l = 0, 1, \dots, d - 1$ in Equation (25).

Theorem 6. Denote, for $i, l, k = 0, \dots, d - 1, c(i, l, k) = \sum_{j=1}^d u_j^{(i)} u_j^{(l)} u_j^{(k)} p_j$, and $u_i = \sum_{j=1}^d u_j^{(i)} x_j, i = 1, \dots, d - 1$. Two recursive systems are:

$$\begin{aligned}
 x_j Q_n(\mathbf{x}; \mathbf{u}) &= \sum_{k=1}^{d-1} (n_k + 1) p_j u_j^{(k)} Q_{n+e_k}(\mathbf{x}; \mathbf{u}) \\
 &+ (N - |\mathbf{n}| + 1) \sum_{l=1}^{d-1} p_j u_j^{(l)} Q_{n-e_l}(\mathbf{x}; \mathbf{u}) \\
 &+ \sum_{l,k=1}^{d-1} (n_k + 1 - \delta_{lk}) p_j u_j^{(l)} u_j^{(k)} Q_{n-e_l+e_k}(\mathbf{x}; \mathbf{u}) + p_j (N - |\mathbf{n}|) Q_n(\mathbf{x}; \mathbf{u}) \quad (49)
 \end{aligned}$$

and:

$$\begin{aligned}
 u_i Q_n(\mathbf{x}; \mathbf{u}) &= (n_i + 1) Q_{n+e_i}(\mathbf{x}; \mathbf{u}) + (N - |\mathbf{n}| + 1) Q_{n-e_i}(\mathbf{x}; \mathbf{u}) \\
 &+ \sum_{l,k=1}^{d-1} c(i, l, k) (n_k + 1 - \delta_{kl}) Q_{n-e_l+e_k}(\mathbf{x}; \mathbf{u}) \quad (50)
 \end{aligned}$$

Proof. Consider:

$$\mathbb{E} \left[X_j G(\mathbf{X}, \mathbf{w}, \mathbf{u}) G(\mathbf{X}, \mathbf{z}, \mathbf{u}) \right] = N p_j \left(1 + \sum_{i=1}^{d-1} w_i u_j^{(i)} \right) \left(1 + \sum_{i=1}^{d-1} z_i u_j^{(i)} \right) \left(1 + \sum_{i=1}^{d-1} w_i z_i \right)^{N-1} \quad (51)$$

Equating coefficients of $\prod_1^{d-1} w_j^{n_j} \prod_1^{d-1} z_j^{n'_j}$;

$$\mathbb{E} \left[X_j Q_n(\mathbf{X}; \mathbf{u}) Q_{n'}(\mathbf{X}; \mathbf{u}) \right] = \begin{cases} \frac{N!}{(N-|\mathbf{n}|-1)! \prod_1^{d-1} n_i!} p_j u_j^{(k)} & \mathbf{n}' = \mathbf{n} + \mathbf{e}_k \\ \frac{N!}{(N-|\mathbf{n}|)! \prod_1^{d-1} n_i!} n_l p_j u_j^{(l)} & \mathbf{n}' = \mathbf{n} - \mathbf{e}_l \\ \frac{N!}{(N-|\mathbf{n}|)! \prod_1^{d-1} n_i!} n_l p_j u_j^{(l)} u_j^{(k)} & \mathbf{n}' = \mathbf{n} - \mathbf{e}_l + \mathbf{e}_k, l \neq k \\ \frac{N!}{(N-|\mathbf{n}|-1)! \prod_1^{d-1} n_i!} p_j + \sum_{l=1}^{d-1} \frac{N!}{(N-|\mathbf{n}|)! \prod_1^{d-1} n_i!} n_l p_j u_j^{(l)2} & \mathbf{n}' = \mathbf{n} \end{cases} \quad (52)$$

The first recursive Equation (49) then follows by an expansion of $x_j Q_n(\mathbf{x}; \mathbf{u})$ as a series in $Q_{n'}(\mathbf{x}; \mathbf{u})$ dividing the cases in Equation (52) to obtain the coefficients by:

$$\binom{N}{\mathbf{n}'+} = \begin{cases} \frac{N!}{(N-|\mathbf{n}|-1)! \prod_1^{d-1} (n_i + \delta_{ik})!} & \mathbf{n}' = \mathbf{n} + \mathbf{e}_k \\ \frac{N!}{(N-|\mathbf{n}|-1)! \prod_1^{d-1} (n_i - \delta_{il})!} & \mathbf{n}' = \mathbf{n} - \mathbf{e}_l \\ \frac{N!}{(N-|\mathbf{n}|)! \prod_1^{d-1} (n_i - \delta_{il} + \delta_{ik})!} & \mathbf{n}' = \mathbf{n} - \mathbf{e}_l + \mathbf{e}_k, l \neq k \\ \frac{N!}{(N-|\mathbf{n}|)! \prod_1^{d-1} n_i!} & \mathbf{n}' = \mathbf{n}. \end{cases} \quad (53)$$

The second recursion Equation (50) is found by summation, using the orthogonality of \mathbf{u} . \square

The dual orthogonal system when \mathbf{u} is orthonormal is:

$$\sum_{\{n \geq 0: |n|=N\}} Q_{n+}(\mathbf{x}; \mathbf{u}) Q_{n+}(\mathbf{x}; \mathbf{u}) \binom{N}{n+}^{-1} = m(\mathbf{x}, \mathbf{p})^{-1} \delta_{xy} \quad (54)$$

A dual generating function is:

$$H(\mathbf{n}, \mathbf{v}, \mathbf{u}) = \sum_{\{\mathbf{x}:|\mathbf{x}|=N\}} \binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} Q_n(\mathbf{x}; \mathbf{u}) \prod_{i=1}^d v_i^{x_i} = \prod_{l=0}^{d-1} \left(\sum_{j=1}^d u_j^{(l)} v_j \right)^{n_l} \tag{55}$$

The generating function Equation (55) arises from considering the coefficient of $\prod_{i=1}^{d-1} w_i^{n_i}$ in:

$$\sum_{\{\mathbf{x}:|\mathbf{x}|=N\}} \binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} G(\mathbf{x}, \mathbf{w}, \mathbf{u}) \prod_{i=1}^d v_i^{x_i} = \binom{N}{\mathbf{n}^+}^{-1} \left(\sum_{j=1}^{d-1} v_j + \sum_{l=1}^{d-1} w_l \sum_{j=1}^d v_j u_j^{(l)} \right)^N \tag{56}$$

Theorem 7. A dual recurrence system is, for $i = 0, \dots, d - 1$:

$$n_i Q_n(\mathbf{x}; \mathbf{u}) = \sum_{j,l=1}^d x_j u_j^{(i)} u_l^{(i)} p_l Q_n(\mathbf{x} - \mathbf{e}_j + \mathbf{e}_l; \mathbf{u}) \tag{57}$$

Proof. A derivation of the recurrence system uses a transform method. Consider:

$$\begin{aligned} & \sum_{\{\mathbf{n}^+;|\mathbf{n}^+|=N\}} n_i \mathbb{E} \left[\prod_{i=1}^d \phi_i^{X_i} \phi_i^{Y_i} Q_n(\mathbf{X}; \mathbf{u}) Q_n(\mathbf{Y}; \mathbf{u}) \right] \binom{N}{\mathbf{n}^+}^{-1} \\ &= N T_i(\boldsymbol{\phi}) T_i(\boldsymbol{\phi}) \left[\sum_{j=1}^d p_j \phi_j \right]^{N-1} \end{aligned} \tag{58}$$

Therefore, non-zero terms with $\mathbf{y} = \mathbf{x} - \mathbf{e}_j + \mathbf{e}_l$ are:

$$\begin{aligned} \sum_{\{\mathbf{n}^+;|\mathbf{n}^+|=N\}} n_i Q_n(\mathbf{x}; \mathbf{u}) Q_n(\mathbf{y}; \mathbf{u}) \binom{N}{\mathbf{n}^+}^{-1} &= \frac{N \binom{N-1}{\mathbf{x}-\mathbf{e}_j} \prod_{k=1}^d p_k^{x_k - \delta_{jk}} p_j u_j^{(i)} p_l u_l^{(i)}}{m(\mathbf{x}, \mathbf{p}) m(\mathbf{y}, \mathbf{p})} \\ &= \frac{x_j u_j^{(i)} p_l u_l^{(i)}}{m(\mathbf{y}, \mathbf{p})} \end{aligned} \tag{59}$$

The dual recurrence is therefore Equation (57). □

The reproducing kernel polynomials:

$$Q_n(\mathbf{x}, \mathbf{y}) = \sum_{\{\mathbf{n}:|\mathbf{n}|=n\}} \binom{N}{\mathbf{n}}^{-1} Q_n(\mathbf{x}; \mathbf{u}) Q_n(\mathbf{y}; \mathbf{u}) \tag{60}$$

are invariant under which set of orthonormal functions \mathbf{u} is used. They have an explicit form; see Diaconis and Griffiths [2] and Xu [7] for details.

3.1. An Ehrenfest Urn with d -Types

A d -type Ehrenfest urn has N balls of d colours $\{1, \dots, d\}$. At rate one, a ball is chosen, and if it is of type j , it is changed to colour l with probability p_{jl} , $l = 1, \dots, d$. $\{\mathbf{X}(t)\}_{t \geq 0}$, with $|\mathbf{X}(t)| = N$, is the number of balls of the different colours at time t , which can be regarded as a d -dimensional random walk on $|\mathbf{x}| = N$. The transition functions have an eigenfunction expansion in the multivariate Krawtchouk polynomials, extending the case Equation (21) with two colours.

Theorem 8. Let $\{X(t)\}_{t \geq 0}$ be a d -dimensional random walk on x , $|x| = N$, where transitions are made from $x \rightarrow x - e_j + e_l$ at rate $r(x, x - e_j + e_l) = (x_j/N)p_{jl}$. P is a $d \times d$ transition matrix, with stationary distribution p , such that:

$$p_{jl} = p_l \left\{ 1 + \sum_{i=1}^{d-1} \rho_i u_j^{(i)} u_l^{(i)} \right\} \tag{61}$$

Then, the transition functions of $X(t)$ have an eigenfunction expansion:

$$p(x, y; t) = m(y, p) \times \left\{ 1 + \sum_{\{n: 0 < |n| \leq N\}} e^{-t \sum_{i=1}^{d-1} n_i(1-\rho_i)/N} \binom{N}{n}^{-1} Q_n(x; u) Q_n(y; u) \right\} \tag{62}$$

Proof. $\{X(t)\}_{t \geq 0}$ is a reversible Markov process with stationary distribution $m(x; p)$, because it satisfies the balance equation:

$$m(x; p)r(x, x - e_j + e_l) = m(x - e_j + e_l; p)r(x - e_j + e_l, x) \tag{63}$$

The reversibility is a consequence of assuming that P is a reversible transition matrix. The generator of the process acting on $f(x)$ is specified by:

$$Lf(x) = \sum_{j,l} r(x, x - e_j + e_l) (f(x - e_j + e_l) - f(x)) \tag{64}$$

so the eigenvalues and eigenvectors $(\lambda_n, g_n(x))$ satisfy:

$$Lg_n(x) = -\lambda_n g_n(x) \tag{65}$$

Now, from Equation (57):

$$-\sum_{i=1}^{d-1} (n_i(1 - \rho_i)/N) Q_n(x; u) = \sum_{j,l=1}^d (x_j/N)p_{jl} Q_n(x - e_j + e_l; u) - Q_n(x; u) \tag{66}$$

which is the same as Equation (65), noting that the total rate is one away from x . Then, Equation (62) holds immediately. \square

3.2. Extensions to the Multivariate Krawtchouk Polynomials

It is useful in considering spectral expansions of composition Markov processes to allow the following generalizations of the multivariate Krawtchouk polynomials.

- Allow $d = \infty$ as a possibility, and let $\{u^{(j)}\}_{j=0}^\infty$ be a complete orthogonal set of functions on p_1, p_2, \dots . The multinomial distribution is still well defined as:

$$m(x; p) = \frac{N!}{x_1! x_2! \dots} p_1^{x_1} p_2^{x_2} \dots, |x| = N \tag{67}$$

and the generating function for the multivariate Krawtchouk polynomials still holds with $d = \infty$.

- When $d = \infty$, take $\{u^{(j)}\}_{j=1}^\infty$ to be orthogonal on a discrete measure π , which is non-negative, but not a probability measure, because $\sum_{i=1}^\infty \pi_i = \infty$.
- Allow the basis functions u to be orthogonal on π , and take the dual functions $\{u_i^{(z)}\}_{i=0}^\infty$ to be orthogonal on a continuous distribution. An example that occurs naturally in composition birth and death chains is when $u_i^{(z)} = L_i^{(\alpha)}(z), z \geq 0, i = 0, 1, \dots$ are the Laguerre polynomials, orthogonal on the density:

$$\frac{z^\alpha}{\Gamma(\alpha + 1)} e^{-z}, z > 0 \tag{68}$$

3.3. Karlin and McGregor Spectral Theory

Consider a birth and death process $\{\xi(t)\}_{t \geq 0}$ on $\{-1, 0, 1, \dots\}$ with birth and death rates λ_i, μ_i from state i and transition probabilities $p_{ij}(t)$. Negative one is an absorbing state, which can be reached if $\mu_0 > 0$. We assume that the process is non-explosive, so only a finite number of events will take place in any finite time interval. Define orthogonal polynomials $\{Q_n(z)\}_{n=0}^\infty$ by:

$$-zQ_n(z) = -(\lambda_n + \mu_n)Q_n(z) + \lambda_n Q_{n+1}(z) + \mu_n Q_{n-1}(z) \tag{69}$$

for $n \in \mathbb{Z}_+$ with $Q_0 = 1$ and $Q_{-1} = 0$. The polynomials are defined by recursion from Equation (69) with Q_{n+1} defined by knowing Q_n and Q_{n-1} . If $\mu_0 = 0$, then $Q_n(0) = 1$. There is a spectral measure ψ with support on the non-negative axis and total mass one, so that:

$$p_{ij}(t) = \pi_j \int_0^\infty e^{-zt} Q_i(z) Q_j(z) \psi(dz) \tag{70}$$

for $i, j = 0, 1, \dots$ where:

$$\pi_j = \frac{\lambda_0 \cdots \lambda_{j-1}}{\mu_1 \cdots \mu_j} \tag{71}$$

If $\mu_0 > 0$, then $\sum_{j=0}^\infty p_{ij}(t) < 1$ because of possible absorption into state -1 . If $\mu_0 = 0$, but there is no stationary distribution, because $\sum_{j=0}^\infty \pi_j = \infty$, then also, possibly, $\sum_{j=0}^\infty p_{ij}(t) < 1$. Placing $t = 0$ shows the orthogonality of the polynomials $\{Q_i(z)\}_{i \geq 0}$ on the measure ψ because $p_{ij}(0) = \delta_{ij}$. $\{\xi(t)\}_{t \geq 0}$ is clearly reversible with respect to $\{\pi_j\}_{j \geq 0}$ when a stationary distribution exists, or before absorption at zero if it does not exist, since $\pi_i p_{ij}(t) = \pi_j p_{ji}(t)$. As $t \rightarrow \infty$ the limit stationary distribution, if $\mu_0 = 0$ and $\sum_{k=0}^\infty \pi_k < \infty$, is:

$$p_j = \frac{\pi_j}{\sum_{k=0}^\infty \pi_k} = \pi_j \psi(\{0\}) \tag{72}$$

Suppose a stationary distribution exists, and there is a discrete spectrum with support $\{\zeta_l\}_{l \geq 0}$, $\zeta_0 = 0$. Then:

$$\begin{aligned} p_{ij}(t) &= \pi_j \sum_{l=0}^\infty e^{-\zeta_l t} Q_i(\zeta_l) Q_j(\zeta_l) \psi(\{\zeta_l\}) \\ &= p_j \left\{ 1 + \sum_{l=1}^\infty e^{-\zeta_l t} Q_i(\zeta_l) Q_j(\zeta_l) \psi(\{\zeta_l\}) / \psi(\{0\}) \right\} \end{aligned} \tag{73}$$

This is an eigenfunction expansion:

$$p_{ij}(t) = p_j \left\{ 1 + \sum_{l \geq 1} e^{-\zeta_l t} u_i^{(l)} u_j^{(l)} \right\}, \quad i, j = 0, 1, \dots \tag{74}$$

where u is a set of orthonormal functions on p defined by:

$$u_i^{(l)} = Q_i(\zeta_l) \sqrt{\psi(\{\zeta_l\}) / \psi(\{0\})}, \quad i, l = 0, 1, \dots \tag{75}$$

Several well-known birth and death processes give rise to classical orthogonal polynomial systems. In this paper, only processes where $\mu_0 = 0$ are considered, so there is no absorbing state at -1 , and the state space is $\{0, 1, \dots\}$. Classical papers where theory is developed and particular spectral expansions Karlin and McGregor [9–11,18]. Schoutens [19] details the birth and death processes and spectral expansions nicely, from which we summarize.

- The $M/M/\infty$ queue where $\lambda_n = \lambda, \mu_n = n\mu, n \geq 0$. The process has a stationary Poisson distribution:

$$p_j = e^{-\lambda/\mu} (\lambda/\mu)^j / j!, j = 0, 1, \dots \tag{76}$$

The orthogonal polynomials are the Poisson–Charlier polynomials:

$$Q_n(z) = C_n(z/\mu; \lambda/\mu), n \geq 0 \tag{77}$$

where $\{C_n(z; \nu)\}_{n=0}^\infty$ has a generating function:

$$\sum_{n=0}^\infty C_n(z; \nu) \frac{w^n}{n!} = e^{w(1-w/\nu)z} \tag{78}$$

- The linear birth and death process where $\lambda_n = (n + \beta)\lambda, \mu_n = n\mu$, with $\lambda, \mu, \beta > 0$. The process arises from individuals which split at rate λ , die at rate μ and immigration of individuals occurs at rate $\lambda\beta$. Then:

$$\pi_j = \frac{\beta^{(j)}}{j!} \left(\frac{\lambda}{\mu}\right)^j, j = 0, 1, \dots \tag{79}$$

There are three cases to consider.

1. $\lambda < \mu$. The spectral polynomials are related to the Meixner polynomials by:

$$Q_n(z) = M_n\left(\frac{z}{\mu - \lambda}; \beta, \frac{\lambda}{\mu}\right), n = 0, 1, \dots \tag{80}$$

The polynomials are orthogonal on:

$$\left(1 - \frac{\lambda}{\mu}\right)^\beta \frac{\beta^{(z)}}{z!} \left(\frac{\lambda}{\mu}\right)^z, z = 0, 1, \dots \tag{81}$$

at points $(\mu - \lambda)z, z = 0, 1, \dots$. The first point of increase is zero corresponding to $e^{0t} = 1$ in the spectrum. There is a negative binomial stationary distribution for the process:

$$p_i = \left(1 - \frac{\lambda}{\mu}\right)^\beta \frac{\beta^{(i)}}{i!} \left(\frac{\lambda}{\mu}\right)^i, i = 0, 1, \dots \tag{82}$$

The Meixner polynomials have a generating function:

$$\sum_{n=0}^\infty M_n(x; a; q) \frac{a^{(n)}}{n!} z^n = (1 - q^{-1}z)^x (1 - z)^{-x-a} \tag{83}$$

2. $\lambda > \mu$.

$$Q_n(z) = \left(\frac{\lambda}{\mu}\right)^n M_n\left(\frac{z}{\lambda - \mu} - \beta; \beta, \frac{\mu}{\lambda}\right), n = 0, 1, \dots \tag{84}$$

The polynomials are orthogonal on:

$$\left(1 - \frac{\mu}{\lambda}\right)^\beta \frac{\beta^{(z)}}{z!} \left(\frac{\mu}{\lambda}\right)^z, z = 0, 1, \dots \tag{85}$$

at points $(z + \beta)(\lambda - \mu), z = 0, 1, \dots$. The first point of increase is $\beta(\lambda - \mu)$, corresponding to a spectral term $e^{-\beta(\lambda - \mu)t}$. There is not a stationary distribution for the process in this case, with $\sum_{j=0}^\infty \pi_j = \infty$.

3. $\lambda = \mu$. The spectral polynomials are related to the Laguerre polynomials by:

$$Q_n(z) = \frac{n!}{\beta^{(n)}} L_n^{(\beta-1)}(z/\lambda), n \geq 0 \tag{86}$$

In this case, there is a continuous spectrum, and the polynomials are orthogonal on the gamma distribution:

$$\frac{1}{\lambda^\beta \Gamma(\beta)} z^{\beta-1} e^{-z/\beta}, z > 0 \tag{87}$$

There is no stationary distribution of the process in this case. The Laguerre polynomials have a generating function:

$$\sum_{n=0}^{\infty} L_n^{(\beta-1)}(x) z^n = (1-z)^{-\beta} \exp\{xz/(1-z)\} \tag{88}$$

- A two-urn model with $\lambda_n = (N-n)(a-n)$, $\mu_n = n(b-(N-n))$, $n = 0, 1, \dots, N$, $a, b \geq N$. The process arises from a model with two urns with a and b balls, with N tagged balls. At an event, two balls are chosen at random from the urns and interchanged. The state of the process is the number of tagged balls in the first urn. The spectral polynomials are related to the dual Hahn polynomials by:

$$Q_n(z) = R_n(\lambda(z); a, b, N), n = 0, 1, \dots \tag{89}$$

where:

$$R_n(\lambda(z); a, b, N) = {}_3F_2(-n, -z, z-a-b-1; -a, -N; 1) \tag{90}$$

orthogonal on:

$$\frac{\binom{N-b-1}{N} N! N_{[z]} a_{[z]} (2z-a-b-1)}{z! b_{[z]} (z-a-b-1)_{(N+1)}} \tag{91}$$

with $\lambda(z) = z(z-a-b-1)$. There is a hypergeometric stationary distribution in the process of:

$$p_i = \frac{\binom{a}{i} \binom{b}{N-i}}{\binom{a+b}{N}}, i = 0, 1, \dots, N \tag{92}$$

- An Ehrenfest urn where $\lambda_n = (N-n)p$, $\mu_n = nq$, $0 \leq n \leq N$, $0 < p < 1$ and $q = 1-p$. The spectral polynomials are the Krawtchouk polynomials:

$$Q_n(z) = K_n(z; N, p), 0 \leq n \leq N \tag{93}$$

orthogonal on the Binomial (N, p) distribution:

$$\binom{N}{z} p^z q^{N-z}, z = 0, 1, \dots, N \tag{94}$$

which is also the stationary distribution in the process.

3.4. Composition Birth and Death Processes

Consider N identically distributed birth and death processes $\{\tilde{\xi}_i(t)\}_{t \geq 0}, i = 1, \dots, N$, each with state space $0, 1, \dots$. It is assumed that there is no absorbing state at -1 and $\lambda_0 > 0$. The transition functions for the labelled processes are $p_{ij}(t) := \prod_{k=1}^N p_{i_k, j_k}(t)$. In composition Markov processes, interest is in the unlabelled configuration of $\xi(t)$ specified by $\mathbf{X}(t)$, where:

$$X_k(t) = |\{i_j = k, j = 1, \dots, N\}| \tag{95}$$

for $k = 0, 1, \dots$. The probability generating function of $\mathbf{X}(t)$ conditional on $\mathbf{X}(0) = \mathbf{x}$ is:

$$\mathbb{E} \left[\prod_{k=1}^d s_k^{X_k(t)} \right] = \prod_{i=0}^d \left(\sum_{j=0}^d p_{ij}(t) s_j \right)^{x_i} \tag{96}$$

where possibly, there is a countable infinity of states with $d = \infty$. Transitions and rates are, for $j = 0, 1, \dots$,

$$x \rightarrow \begin{cases} x + e_{j+1} - e_j & \text{rate } x_j \lambda_j, \\ x + e_{j-1} - e_j & \text{rate } x_j \mu_j. \end{cases} \tag{97}$$

The total rate from x is $\sum_{j \geq 0} x_j (\lambda_j + \mu_j)$. $\{X(t)\}_{t \geq 0}$ is reversible with respect to $\tilde{m}(x; \pi) = \binom{N}{x} \prod_{j=1}^d \pi_j^{x_j}$ in the sense that:

$$\begin{aligned} \tilde{m}(x; \pi) \lambda_j x_j &= \tilde{m}(x + e_j; \pi) \mu_{j+1} x_{j+1}, \quad j = 0, 1, \dots \\ \tilde{m}(x; \pi) \mu_j x_j &= \tilde{m}(x - e_j; \pi) \lambda_{j-1} x_{j-1}, \quad j = 1, 2, \dots \end{aligned} \tag{98}$$

Theorem 9. If the spectrum is discrete, with support $\{\zeta_l\}_{l \geq 0}$, $\mu_0 = 0$, $\zeta_0 = 0$, and a stationary distribution exists, then:

$$p(x, y; t) = m(y, p) \left\{ 1 + \sum_{\{n: 0 < |n| \leq N\}} e^{-t \sum_{i \geq 1} n_i \zeta_i} \binom{N}{n}^{-1} Q_n(x; u) Q_n(y; u) \right\} \tag{99}$$

where $\{Q_n(x; u)\}$ are the multivariate Krawtchouk polynomials with:

$$u_i^{(l)} = Q_i(\zeta_l) \sqrt{\psi(\zeta_l) / \psi(0)}, \quad i, l = 0, 1, \dots \tag{100}$$

The indexing in elements of x, y now begins at zero. If the spectrum is discrete, with support $\{\zeta_l\}_{l \geq 0}$, $\mu_0 = 0$, then:

$$p(x, y; t) = \tilde{m}(y; \pi) \sum_{\{n: 0 \leq |n| \leq N\}} e^{-t \sum_{i \geq 0} n_i \zeta_i} \binom{N}{n}^{-1} Q_n(x; u) Q_n(y; u) \tag{101}$$

where $\{Q_n(x; u)\}$ are the multivariate Krawtchouk polynomials with:

$$u_i^{(l)} = Q_i(\zeta_l) \sqrt{\psi(\zeta_l)}, \quad i, l = 0, 1, \dots \tag{102}$$

In this case, $\zeta_0 > 0$, $u^{(0)}$ is not identically one, and:

$$\sum_{i \geq 0} u_i^{(k)} u_i^{(l)} \pi_i = \delta_{kl}, \quad k, l = 0, 1, \dots \tag{103}$$

This covers the case when a stationary distribution does exist and also when a stationary distribution does not exist, because $\sum_{k=0}^{\infty} \pi_k = \infty$.

Proof. The probabilistic structure of $\{X(t)\}_{t \geq 0}$ with probability-generating function Equation (96) implies that the multivariate Krawtchouk polynomials are the eigenfunctions of the transition distribution. Indexing in $X(t)$ is from zero, rather than the usual indexing from one. From the Karlin and McGregor spectral expansion Equation (70):

$$\begin{aligned} p_{ij}(t) &= \pi_j \left\{ \sum_{k \geq 0} e^{-t \zeta_k} Q_i(\zeta_k) Q_j(\zeta_k) \psi(\{\zeta_k\}) \right\} \\ p_{ij}(t) &= \psi(\{0\}) \pi_j \left\{ 1 + \sum_{k \geq 1} e^{-t \zeta_k} Q_i(\zeta_k) Q_j(\zeta_k) \psi(\{\zeta_k\}) / \psi(\{0\}) \right\} \\ &= p_j \left\{ 1 + \sum_{k \geq 1} e^{-t \zeta_k} u_i^{(k)} u_j^{(k)} \right\} \end{aligned} \tag{104}$$

where $\{u_i^{(k)}\}$ is defined in Equation (100) and satisfies:

$$\sum_{i \geq 0} u_i^{(k)} u_i^{(l)} p_i = \delta_{kl}, \quad k, l \geq 0 \tag{105}$$

The second case Equation (101) follows similarly. The multivariate Krawtchouk polynomials then have a generating function:

$$G(\mathbf{x}, \mathbf{w}, \mathbf{u}) = \prod_{j \geq 0} \left(u_j^{(0)} + \sum_{l \geq 1} w_l u_j^{(l)} \right)^{x_j}. \tag{106}$$

□

The transition probability expansion Equation (101) can be written in a Karlin and McGregor spectral expansion form where the dual polynomials are important. Denote $\tilde{u}_i^{(l)} = Q_i(\zeta_l), i, l = 0, 1, \dots;$ $Q_x(\mathbf{v}; \tilde{\mathbf{u}}) = \binom{N}{\mathbf{v}}^{-1} Q_{\mathbf{v}}(\mathbf{x}; \tilde{\mathbf{u}});$ and a multinomial spectral measure (which is a probability measure):

$$\tilde{m}(\mathbf{v}; \psi) = \binom{N}{\mathbf{v}} \psi(\zeta_0)^{v_0} \psi(\zeta_1)^{v_1} \dots, \quad v_0 + v_1 + \dots = N \tag{107}$$

Then, Equation (101) can be expressed as a spectral expansion:

$$p(\mathbf{x}, \mathbf{y} : t) = \tilde{m}(\mathbf{y}; \boldsymbol{\pi}) \sum_{\{\mathbf{v}; 0 \leq |\mathbf{v}| \leq N\}} e^{-t \sum_{i \geq 0} v_i \zeta_i} Q_x(\mathbf{v}; \tilde{\mathbf{u}}) Q_y(\mathbf{v}; \tilde{\mathbf{u}}) \tilde{m}(\mathbf{v}; \psi) \tag{108}$$

The generating function of the dual polynomials:

$$\begin{aligned} H(\mathbf{n}, \mathbf{v}, \tilde{\mathbf{u}}) &= \sum_{\{\mathbf{x}; |\mathbf{x}|=N\}} \binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} Q_{\mathbf{n}}(\mathbf{x}, \tilde{\mathbf{u}}) \prod_{i \geq 0} v_i^{x_i} \\ &= \prod_{l \geq 0} \left(v_0 + \sum_{j \geq 1} Q_j(\zeta_l) v_j \right)^{n_l} \\ &= \prod_{k=1}^N \left(v_0 + \sum_{j \geq 1} Q_j(Z_k) v_j \right) \end{aligned} \tag{109}$$

where in this generating function $\mathbf{n}(\mathbf{Z})$ is regarded as a random variable by taking:

$$n_l(\mathbf{Z}) = |\{Z_k : Z_k = \zeta_l, k = 1, \dots, N\}| \tag{110}$$

$\{Z_k\}_{k=1}^N$ are independent and identically distributed random variables with probability measure ψ . Without loss of generality, take $v_0 = 1$ in Equation (109) and consider coefficients of $\prod_{i \geq 1} v_i^{x_i}$, indexing the dual polynomial by (x_1, x_2, \dots) with $x_1 + x_2 + \dots \leq N$. Note the scaling that the dual polynomials is one when $x_i = 0, i \geq 1$.

Theorem 10. Define:

$$\mathcal{N}_j = \sum_{k=1}^N Q_j(Z_k) = \sum_{l \geq 0} n_l Q_j(\zeta_l), \quad j \geq 1 \tag{111}$$

$\binom{N}{\mathbf{n}^+}^{-1} Q_{\mathbf{n}}(\mathbf{x}, \tilde{\mathbf{u}})$ is a polynomial of degree $x_1 + x_2 + \dots$ in $\{\mathcal{N}_j\}_{j \geq 1}$ whose only term of maximal degree is $\prod_{j \geq 1} \mathcal{N}_j^{x_j}$. The total degree of \mathbf{Z} in the dual polynomials indexed by (x_1, x_2, \dots) is $\sum_{j \geq 1} j x_j$ with a single leading term of this degree.

Proof. The proof of the first statement follows from Theorem 5. The proof of the second statement is immediate by knowing that \mathcal{N}_j is of degree j in \mathbf{Z} . □

The third case of linear birth and death processes' composition Markov chains is interesting, as it has a continuous spectral measure, which is a product measure of N gamma distribution measures. The spectral polynomials are well defined by a generating function as coefficients of $\prod_{j=1}^{\infty} v_j^{x_j}$ in:

$$\prod_{k=1}^N \left(1 + \sum_{j \geq 1} Q_j(Z_k) v_j \right) \quad (112)$$

however, elements of $\{Z_k\}_{k=1}^N$ are distinct, being continuous random variables, and the dual of the dual system is the products of dual Laguerre polynomials, which are not grouped to an index n , as when there is a discrete spectrum.

The polynomials in the Meixner class Equation (3) are additive in the sense that if $\{Q_m^N(|z|)\}$ are the orthogonal polynomials on the distribution of $|Z|$, then the generating function for these polynomials is:

$$G^N(v, |z|) = h(v)^N e^{|z|u(v)} = \sum_{m=0}^{\infty} Q_m^N(|z|) v^m / m! \quad (113)$$

and:

$$Q_m^N(|z|) = \sum_{\{m: |m|=m\}} \binom{m}{\mathbf{m}} \prod_{j=1}^N Q_{m_j}(z_j) \quad (114)$$

This additivity implies an interesting identity.

Theorem 11. The dual multivariate Krawtchouk polynomials with generating function Equation (109) satisfy the identity:

$$\binom{N}{\mathbf{n}}^{-1} \sum_{\{x: \sum_{j=1}^{\infty} j x_j = m\}} \binom{N}{\mathbf{x}} \frac{m!}{\prod_{j=1}^{\infty} j!^{x_j}} Q_n(\mathbf{x}, \tilde{\mathbf{n}}) = Q_m^N(|Z|) \quad (115)$$

where $\mathbf{x} = (x_1, x_2, \dots)$. In this equation, $\mathbf{n} = \mathbf{n}(Z)$ is regarded as a random variable in the sense of Equation (110).

Proof. Set $v_j = v^j / j!$, $j = 0, 1, \dots$ in Equation (109). Then:

$$\begin{aligned} \sum_{\{x: |x|=N\}} \binom{N}{\mathbf{n}^+}^{-1} \binom{N}{\mathbf{x}} Q_n(\mathbf{x}, \tilde{\mathbf{n}}) \frac{v^{\sum_{j=1}^{\infty} j x_j}}{\prod_{j=1}^{\infty} j!^{x_j}} &= \prod_{k=1}^N \left(\sum_{j \geq 0} Q_j(Z_k) v^j / j! \right) \\ &= h(v)^N e^{|Z|u(v)} \\ &= \sum_{m=0}^{\infty} Q_m^N(|Z|) v^m / m! \end{aligned} \quad (116)$$

The theorem then follows by equating coefficients of v^m on both sides of the generating function. \square

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