Communications on Stochastic Analysis
Vol. 10, No. 3 (2016) 297-320

Serials Publications
www.serialspublications.com

KRAWTCHOUK-GRIFFITHS SYSTEMS I: MATRIX APPROACH

PHILIP FEINSILVER

Abstract. We call *Krawtchouk-Griffiths* systems, or KG-systems, systems of multivariate polynomials orthogonal with respect to corresponding multinomial distributions. The original Krawtchouk polynomials are orthogonal with respect to a binomial distribution. Our approach is to work directly with matrices comprising the values of the polynomials at points of a discrete grid based on the possible counting values of the underlying multinomial distribution. The starting point for the construction of a KG-system is a *generating matrix* satisfying the K-condition, orthogonality with respect to the basic probability distribution associated to an individual step of the multinomial process. The variables of the polynomials corresponding to matrices may be interpreted as quantum observables in the real case, or quantum variables in the complex case. The structure of the recurrence relations for the orthogonal polynomials is presented with multiplication operators as the matrices corresponding to the quantum variables. An interesting feature is that the associated random walks correspond to the Lie algebra of the representation of symmetric tensor powers of matrices.

1. Introduction

The original paper of Krawtchouk [14] presents polynomials orthogonal with respect to a general binomial distribution and discusses the connection with Hermite polynomials.

Group-theoretic approaches have been presented by Koornwinder [13] for the on-variable case. Kocik [12] emphasises a geometric approach, mainly from the perspective of Lie group actions while a "path integral" approach is presented there as well for the binomial case.

We developed the viewpoint [4] of matrices, noticed in the work of N. Bose [1] for the binomial case, with entries the values of Krawtchouk polynomials on their domain. Matrix constructions for the multivariate case basic to this work were presented in [6], acknowledging the foundational work of Griffiths, see [2, 7, 8, 9], also [15]. Another point of view, the analytic and quantization aspects, is that of "Bernoulli systems", based on the approach of [5]. See [10, 11] for probabilistic aspects as well.

Received 2012-12-6; Communicated by A. Boukas.
2010 *Mathematics Subject Classification.* Primary 15A69, 15A72, 42C05; Secondary 20H20, 22E60.
Key words and phrases. Orthogonal polynomials, multivariate polynomials, Krawtchouk polynomials, symmetric tensor powers, symmetric representation, discrete quantum systems, Kravchuk matrices, multinomial distribution.

The symmetric representation, the action of operators on symmetric tensor space, is a main part of invariant theory. See [16] in the context of coding theory and for the invariant theory setting [17], e.g. The infinite dimensional version, boson Fock space, is fundamental in the second quantization of operators in quantum theory and is a major component of quantum probability theory.

Important aspects of this work include a general recurrence formula for symmetric representations in Section 2. The Transpose Lemma plays an essential rôle in this work. The vector field formulation and Lie algebra maps are standard constructions, newly appearing in this context, see [12], important to our approach. The Columns Theorem and quantum variables comprise Sections 3 and 4. The term "quantum variable" is used to signify unitary equivalence to a diagonal matrix, but the spectrum may not be entirely real. Multivariate Krawtchouk polynomials make their appearance in Section 5 with quantum variables providing recurrence formulas and linearization formulas. We conclude after a section with important examples, especially properties involving reflections.

1.1. Basic notations and conventions.

(1) We consider polynomials in $d+1$ commuting variables over a field, which we typically take to be $\mathbb{C}$, while the constructions are valid over $\mathbb{R}$ as well.

(2) Multi-index notations for powers. With $n = (n_0, \ldots, n_d)$, $x = (x_0, \ldots, x_d)$:

$$x^n = x_0^{n_0} \cdots x_d^{n_d}$$

and the total degree $|n| = \sum_i n_i$. Typically m and n will denote multi-indices, with i, j, k, l for single indices. Running indices may be used as either type, determined from the context.

(3) Vectors, conventionally taken to be column vectors, will be indicated by boldface, with components as usual, e.g.,

$$\mathbf{v} = \begin{pmatrix} v_0 \\ v_1 \\ \vdots \\ v_d \end{pmatrix} .$$

(4) We use the following *summation convention*

repeated Greek indices, e.g., λ or μ, are summed from 0 to d.

Latin indices i, j, k, run from 0 to d and are summed only when explicitly indicated.

(5) For simplicity, we will always denote identity matrices of the appropriate dimension by I.

The transpose of a matrix A is denoted $A^\top$, with Hermitian transpose A^*. The inner product $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^* \mathbf{w}$. The dot product $\mathbf{v} \cdot \mathbf{w} = \sum v_i w_i = v_\lambda w_\lambda$.

We will use the notation U to denote an arbitrary unitary matrix, orthogonal in the real case, i.e., it is a unitary map with respect to the standard inner product.

(6) Given $N \geq 0$, B is defined as the multi-indexed matrix having as its only non-zero entries

$$B_{mm} = \binom{N}{m} = \frac{N!}{m_0! \dots m_d!}$$

the multinomial coefficients of order N.

(7) For a tuple of numbers, diag$(\dots)$ is the diagonal matrix with the tuple providing the entries forming the main diagonal.

(8) The bar notation, $A \to \bar{A}$, is only used for the symmetric power mapping, with complex conjugation indicated by (included in) the star, $z \to z^*$.

2. Symmetric Powers of Matrices

2.1. Basic construction and properties. Given a $(d+1) \times (d+1)$ matrix, A, as usual, $(Ax)_i = \sum_j A_{ij} x_j$. For integer $N \geq 0$, we have the matrix elements, $\bar{A}$, of the symmetric representation of A in degree N defined by the relations

$$(Ax)^m = \sum_n \bar{A}_{mn} x^n \tag{2.1}$$

where we typically drop explicit indication of N if it is understood from the relations $N = |m| = |n|$, noting that $\bar{A}_{mn} = 0$ unless $|m| = |n|$. Monomials are ordered according to dictionary ordering with 0 ranking first, followed by $1, 2, \dots, d$. Thus the first column of $\bar{A}$ gives the coefficients of x_0^N, etc.

In degree N, we have the trace of $\bar{A}$

$$\operatorname{tr}_{\mathrm{Sym}}^{N} A = \sum_m \bar{A}_{mm} \ .$$

For $N = 0$, $\bar{A}_{00} = \operatorname{tr}_{\mathrm{Sym}}^{0} A = 1$, for any matrix A.

Remark 2.1*.* If we require the degree to be indicated explicitly we write $\bar{A}^{(N)}$ accordingly.

2.1.1. *Homomorphism property.* Successive application of B then A shows that this is a homomorphism of the multiplicative semigroup of square $(1+d) \times (1+d)$ matrices into the multiplicative semigroup of square $\binom{N+d}{N} \times \binom{N+d}{N}$ matrices. We call this the **symmetric representation** of the multiplicative semigroup of matrices. In particular, it is a representation of $\mathrm{GL}(d+1)$ as matrices in $\mathrm{GL}(\nu)$, with $\nu = \binom{N+d}{N}$.

Proposition 2.2. *Matrix elements satisfy the homomorphism property*

$$\overline{AB}_{mn} = \sum_k \bar{A}_{mk} \bar{B}_{kn} \ .$$

Proof. Let $y = (AB)x$ and $w = Bx$. Then,

$$\begin{aligned} y^m &= \sum_n \overline{AB}_{mn}\, x^n \\ &= \sum_k \bar{A}_{mk}\, w^k \\ &= \sum_n \sum_k \bar{A}_{mk} \bar{B}_{kn}\, x^n \ . \end{aligned}$$

□

Remark 2.3. It is important to note that the bar mapping is *not* linear, neither homogeneous nor additive. For example, for $N > 1$,

$$\overline{X + X} = \overline{2X} = 2^N \bar{X} \neq 2\,\bar{X} \ .$$

2.1.2. *Transpose Lemma.* Here we show the relation between $\overline{A^\top}$ and $\bar{A}^\top$. The idea is to consider the polynomial bilinear form $\sum\limits_{i,j} x^i A_{ij} y^j$ and its analogous forms in degrees $N > 0$. The multinomial expansion yields

$$\Big(\sum_{i,j} x^i A_{ij} y^j\Big)^N = \sum_m x^m \binom{N}{m} (Ay)^m = \sum_m x^m \binom{N}{m} \bar{A}_{mn} y^n \qquad (2.2)$$

for degree N.

Replacing A by $A^\top$ yields

$$\Big(\sum_{i,j} x^i A_{ji} y^j\Big)^N = \sum_{m,n} x^m \binom{N}{m} \overline{A^\top}_{mn} y^n$$

which, interchanging indices i and j, equals

$$\begin{aligned} \Big(\sum_{i,j} y^i A_{ij} x^j\Big)^N &= \sum_{m,n} y^m \binom{N}{m} \overline{A}_{mn} x^n = \sum_{m,n} x^m \binom{N}{n} \overline{A}_{nm} y^n \\ &= \sum_{m,n} x^m \binom{N}{n} \bar{A}^\top_{mn} y^n \end{aligned}$$

exchanging indices m and n. Comparing shows that

$$\overline{A^\top}_{mn} = \binom{N}{m}^{-1} \binom{N}{n} \bar{A}^\top_{mn}$$

In terms of B, we see that

Lemma 2.4. Transpose Lemma
The symmetric representation satisfies

$$\overline{A^\top} = B^{-1} \bar{A}^\top B$$

and similarly for adjoints

$$\overline{A^*} = B^{-1} \bar{A}^* B \ .$$

Remark 2.5. (*Diagonal matrices and trace*) Note that the N^{th} symmetric power of a diagonal matrix, D, is itself diagonal with homogeneous monomials of the entries of the original matrix along its diagonal. In particular, the trace will be the N^{th} homogeneous symmetric function in the diagonal entries of D.

Example 2.6. For $V = \begin{pmatrix} v_0 & 0 & 0 \\ 0 & v_1 & 0 \\ 0 & 0 & v_2 \end{pmatrix}$ we have

$$\bar{V}^{(2)} = \begin{pmatrix} v_0^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_0v_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & v_0v_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & v_1^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & v_1v_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & v_2^2 \end{pmatrix}$$

and so on .

2.2. General recurrence formulas. Let R be a $(d+1) \times (d+1)$ matrix. Let $\bar{R}^{(N-1)}$ and $\bar{R}^{(N)}$ denote the matrices of the symmetric tensor powers of R in degrees $N-1$ and N respectively.

Recall the usage e_i for a standard multi-index corresponding to the standard basis vector e_i, $0 \le i \le d$.

First some useful operator calculus.

2.2.1. *Boson operator relations.* Let $\partial_i = \frac{\partial}{\partial x_i}$ and ξ_i denote the operators of partial differentiation with respect to x_i and multiplication by x_i respectively. The basic commutation relations

$$[\partial_i, \xi_j] = \delta_{ij} 1$$

extend to polynomials $f(x)$

$$[\partial_i, f(\xi)] = \frac{\partial f}{\partial x_i} 1$$

With $\partial_i 1 = 0$, $\forall i$, we write

$$\partial_i f(\xi) 1 = \partial_i f(x) = \frac{\partial f}{\partial x_i}$$

evaluating as functions of x as usual.

Now observe that if R is a matrix with inverse S, then

$$[\partial_\lambda S_{\lambda i}, R_{j\mu}\xi_\mu] = \delta_{ij} 1$$

i.e. $(\partial)S$ and $R\xi$ satisfy the boson commutation relations. Hence $(\partial)S$ will act as partial differentiation operators on the variables Rx.

Remark 2.7. For brevity, we write $(\partial)S$ as ∂S, where it is understood that the ∂ symbol stands for the tuple $(\partial_0, \ldots, \partial_d)$ and is not acting on the matrix S.

We will use these observations to derive recurrence relations for matrix elements of the symmetric representation.

Proposition 2.8. *Let m be a multi-index with $|m| = N$ and n be a multi-index with $|n| = N-1$. Then we have the recurrence relation*

$$\sum_{k=0}^{d} m_k\, \bar{R}^{(N-1)}_{m-e_k,n} R_{kj} = (n_j+1)\bar{R}^{(N)}_{m,n+e_j}\ .$$

Proof. Starting from $(Rx)^m$, use the boson commutation relations

$$[(\partial S)_i, (R\xi)_j] = \delta_{ij} I$$

where $S = R^{-1}$. We have, evaluating as functions of x,

$$(\partial S)_i (Rx)^m = m_i (Rx)^{m-e_i} = \sum_n m_i \bar{R}_{m-e_i,n} x^n$$

and directly

$$\partial_\lambda S_{\lambda i} \sum_n \bar{R}_{mn} x^n = S_{\lambda i} \sum_n \bar{R}_{mn} n_\lambda x^{n-e_\lambda}\ .$$

Shifting the index in this last expression and comparing coefficients with the previous line yields

$$m_i \bar{R}_{m-e_i,n} = S_{\lambda i} \bar{R}_{m,n+e_\lambda}(n_\lambda + 1)$$

Now multiply both sides by R_{ij} and sum over i to get the result (with k replacing the running index i). □

2.3. Vector field generating the action of a matrix. We consider the case where

$$R = e^g$$

for $g \in \mathfrak{gl}(d+1)$. Recall the method of characteristics:

For a vector field $H = a(x)\cdot\partial = a(x)_\lambda \partial_\lambda$, the solution to

$$\frac{\partial u}{\partial t} = Hu$$

with initial condition $u(x,0) = f(x)$ is given by the exponential

$$u(x,t) = \exp(tH) f(x) = f(x(t))$$

where $x(t)$ satisfies the autonomous system

$$\dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t} = a(x)$$

with initial condition $x(0) = x$. Note that $a(x)$ on the right-hand side means $a(x(t))$ with t implicit.

Now consider

$$H = gx\cdot\partial = g_{\mu\lambda} x_\lambda \partial_\mu$$

We have the characteristic equations

$$\dot{x} = gx$$

with initial condition $x(0) = x$. The solution is the matrix exponential

$$x(t) = e^{tg} x$$

which we can write as

$$x(t) = R^t x\ .$$

Hence

Proposition 2.9. *For $R = e^g$, we have the one-parameter group action*

$$\exp(t\,gx \cdot \partial)f(x) = f(R^t x)\ .$$

In particular, we have the action of R

$$\exp(gx \cdot \partial)f(x) = f(Rx)\ .$$

2.4. Gamma maps. Let ϕ be any smooth homomorphism of matrix Lie groups. Then the image

$$\phi(e^{tX})$$

of the one-parameter group $\exp(tX)$ is a one -parameter group as well. We define its generator to be

$$\Gamma_\phi(X)$$

That is,

$$\phi(e^{tX}) = e^{t\,\Gamma_\phi(X)}\ .$$

In other words,

$$\Gamma_\phi(X) = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_0 \phi(e^{tX}) = \phi'(I)X$$

by the chain rule, where ϕ' is the jacobian of the map ϕ. Hence

Proposition 2.10. *The gamma map determined by the relation*

$$\phi(e^{tX}) = e^{t\,\Gamma_\phi(X)}$$

can be computed as

$$\Gamma_\phi(X) = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_0 \phi(I + tX)$$

the directional derivative of ϕ at the identity in the direction X.

This provides a convenient formulation that is useful computationally as well as theoretically.

Remark 2.11. We denote the gamma map for the symmetric representation simply by $\Gamma(X)$. The properties of the gamma map as a Lie homomorphism are shown in the Appendix.

The main result we will use for KG-systems follows:

Corollary 2.12.
Given matrices $Y_1, \ldots, Y_s$. The coefficient of v_j in $\overline{I + \sum_j v_j Y_j}$ is $\Gamma(Y_j)$. That is,

$$\overline{I + \sum_j v_j Y_j} = I + \sum_j v_j \Gamma(Y_j) + [\textit{higher order terms in } v_j\textit{'s}]$$

Proof. Introduce the factor t. By linearity,

$$\overline{I + t\sum_j v_j Y_j} = I + t\sum_j v_j \Gamma(Y_j) + t^2(\ldots)$$

where t^2 multiplies the terms higher order in the v's. Setting $t = 1$ yields the result. ∎

The Transpose Lemma applies to the gamma map as follows:

Proposition 2.13. *Under the* Γ*-map the Hermitian transpose satisfies*

$$\Gamma(X^*) = B^{-1}\Gamma(X)^* B \ .$$

Proof. Write

$$\overline{X^*} = B^{-1}\bar{X}^* B$$

Exponentiating:

$$\begin{aligned} e^{t\Gamma(X^*)} &= \overline{e^{tX^*}} = \overline{(e^{tX})^*} \\ &= B^{-1}\overline{e^{tX}}^* B = B^{-1}e^{t\Gamma(X)^*}B \end{aligned}$$

differentiating with respect to t at 0 yields the result. □

2.4.1. *Gamma map for symmetric representation.* For the symmetric representation, take $f = x^m$ in the above Proposition. We have

$$\begin{aligned} \exp(t\, gx\cdot\partial)x^m &= \sum_n (\overline{e^{tg}})_{mn} x^n \\ &= \sum_n (e^{t\Gamma(g)})_{mn} x^n \ . \end{aligned}$$

Now differentiate with respect to t at $t = 0$ to get

$$(gx\cdot\partial)x^m = \sum_n \Gamma(g)_{mn} x^n$$

The left-hand side is

$$g_{\mu\lambda}x_\lambda\partial_\mu x^m = \sum_{j,k} g_{kj} m_k x^{m-e_k+e_j}$$

Hence

Proposition 2.14. *The entries of* $\Gamma(g)$ *are given by*

$$\Gamma(g)_{mn} = \sum_{\substack{0\le i,j\le d \\ n=m-e_i+e_j}} m_i\, g_{ij} \ .$$

Remark 2.15. (*Diagonal matrices and trace*) The gamma map for a diagonal matrix will be diagonal with entries sums of choices of N of the entries of the original matrix corresponding to the monomials of the symmetric power. The trace turns out to be

$$\operatorname{tr}\Gamma(X) = \binom{N+d}{d+1}\operatorname{tr} X \ .$$

Example 2.16. For $V = \begin{pmatrix} v_0 & 0 & 0 \\ 0 & v_1 & 0 \\ 0 & 0 & v_2 \end{pmatrix}$ we have, for $d = 2$, $N = 2$,

$$\Gamma(V) = \begin{pmatrix} 2v_0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_0 + v_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & v_0 + v_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2v_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & v_1 + v_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2v_2 \end{pmatrix}$$

and so on .

3. Columns Theorem and Quantum Variables

Given a matrix A, with each column of A form a diagonal matrix. Thus,

$$\Lambda_j = \operatorname{diag}\left((A_{ij})\right)$$

that is,

$$(\Lambda_j)_{ii} = A_{ij} \ .$$

Theorem 3.1. Columns Theorem. *For any matrix A, let Λ_j be the diagonal matrix formed from column j of A. Let*

$$\Lambda = \sum v_j \Lambda_j \ .$$

Then the coefficient of v^n in the level N induced matrix $\bar{\Lambda}$ is a diagonal matrix with entries the n^{th} column of $\bar{A}$.

Proof. Setting $y = \Lambda x$, we have

$$y_k = \Bigl(\sum v_j A_{kj}\Bigr) x_k \ \Rightarrow \ y^m = \Bigl(\sum \bar{A}_{mn} v^n\Bigr) x^m \ .$$

A careful reading of the coefficients yields the result. □

We may express this in the following useful way: *the diagonal entries of $\bar{\Lambda}$ are generating functions for the matrix elements of $\bar{A}$* . And we have

Corollary 3.2. *Let A be such that the first column, label 0, consists of all 1's. Then with Λ_j as in the above theorem, we have*

$$\operatorname{diag}(\textit{column } j \textit{ of } \bar{A}) = \Gamma(\Lambda_j)$$

for $1 \le j \le d$.

Proof. In the Columns Theorem we have

$$\Lambda = v_0 I + \sum_{1 \le j \le d} v_j \Lambda_j \ .$$

The leading monomials are v_0^N, $v_0^{N-1} v_1$,…,$v_0^{N-1} v_d$. These multiply diagonal matrices with entries the first $1 + d$ columns of $\bar{A}$ respectively. Now let $v_0 = 1$. By Corollary 2.12 we have the coefficients of v_1 through v_d given by the diagonal matrices $\Gamma(\Lambda_j)$, $1 \le j \le d$. Combining these two observations yields the result. □

Example 3.3. Let $A = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}$. We have

$$\Lambda_0 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad , \qquad \Lambda_1 = \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix}$$

and

$$\Lambda = \begin{pmatrix} v_1 + 3v_2 & 0 \\ 0 & 2v_1 + 4v_2 \end{pmatrix}$$

We have

$$\bar{A}^{(2)} = \begin{pmatrix} 1 & 6 & 9 \\ 2 & 10 & 12 \\ 4 & 16 & 16 \end{pmatrix}$$

and

$$\bar{\Lambda}^{(2)} = \begin{pmatrix} v_0^2 + 6v_0v_1 + 9v_1^2 & 0 & 0 \\ 0 & 2v_0^2 + 10v_0v_1 + 12v_1^2 & 0 \\ 0 & 0 & 4v_0^2 + 16v_0v_1 + 16v_1^2 \end{pmatrix}$$

Example 3.4. Now consider $A = \begin{pmatrix} 1 & a & d \\ 1 & b & e \\ 1 & c & f \end{pmatrix}$, here a, b, c, d, e, f are arbitrary numbers. We have

$$\Lambda_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad , \qquad \Lambda_1 = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \quad , \qquad \Lambda_2 = \begin{pmatrix} d & 0 & 0 \\ 0 & e & 0 \\ 0 & 0 & f \end{pmatrix} \quad .$$

with

$$\bar{A}^{(2)} = \begin{pmatrix} 1 & 2a & 2d & a^2 & 2ad & d^2 \\ 1 & a+b & d+e & ab & ae+bd & de \\ 1 & a+c & d+f & ac & af+cd & df \\ 1 & 2b & 2e & b^2 & 2be & e^2 \\ 1 & b+c & e+f & bc & bf+ce & ef \\ 1 & 2c & 2f & c^2 & 2cf & f^2 \end{pmatrix}$$

and

$$\Gamma(\Lambda_1) = \begin{pmatrix} 2a & 0 & 0 & 0 & 0 & 0 \\ 0 & a+b & 0 & 0 & 0 & 0 \\ 0 & 0 & a+c & 0 & 0 & 0 \\ 0 & 0 & 0 & 2b & 0 & 0 \\ 0 & 0 & 0 & 0 & b+c & 0 \\ 0 & 0 & 0 & 0 & 0 & 2c \end{pmatrix}$$

$$\Gamma(\Lambda_2) = \begin{pmatrix} 2d & 0 & 0 & 0 & 0 & 0 \\ 0 & d+e & 0 & 0 & 0 & 0 \\ 0 & 0 & d+f & 0 & 0 & 0 \\ 0 & 0 & 0 & 2e & 0 & 0 \\ 0 & 0 & 0 & 0 & e+f & 0 \\ 0 & 0 & 0 & 0 & 0 & 2f \end{pmatrix}$$

accordingly.

4. Associated and Quantum Variables

Recall that in the finite-dimensional case, quantum observables are Hermitian matrices, thus unitarily equivalent to a real diagonal matrix.

Let A satisfy the condition that its first column consists of all 1's. Form Λ_j from A as in the Columns Theorem. Define, for each j,

$$X_j = A^{-1}\Lambda_j A \ .$$

For X_j so defined, we have the following terminology.

Definition 4.1. Given A. Define an *associated variable* to be a matrix equivalent to a diagonal matrix with A as similarity transformation, where the entries of the diagonal matrix are from a column of A.

If it turns out that this yields a unitary equivalence, for complex A, we call them *quantum variables.* For real A, they will be quantum observables.

Remark 4.2. Note that our standard choice of A will have Λ_0 always equal to the identity matrix and hence the same for X_0.

Set $X = \sum v_j X_j$. Then with Λ as in the Columns Theorem, we have the spectral relations

$$AX = \Lambda A$$
$$Ae^{tX} = e^{t\Lambda}A$$

barring and taking derivatives at 0 yields $\bar{A}\Gamma(X) = \Gamma(\Lambda)\bar{A}$. Taking adjoints we have

$$\Gamma(X)^*(\bar{A})^* = (\bar{A})^*\Gamma(\Lambda)^* \tag{4.1}$$

with columns of $(\bar{A})^*$ eigenvectors of $\Gamma(X)^*$, i.e., this is a spectral resolution of $\Gamma(X)^*$. By Corollary 3.2, the corresponding eigenvalues are complex conjugates of the entries of the columns of $\bar{A}$. For real A we have real spectra and hence quantum observables.

Example 4.3. Take $A = \begin{pmatrix} 1 & 3 \\ 1 & 4 \end{pmatrix}$. We have

$$\Lambda_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ , \qquad \Lambda_1 = \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} \ .$$

With X_0 the identity, we have

$$X_1 = \begin{pmatrix} 0 & -12 \\ 1 & 7 \end{pmatrix} \qquad \text{and} \qquad \Gamma(X_1) = \begin{pmatrix} 0 & -24 & 0 \\ 1 & 7 & -12 \\ 0 & 2 & 14 \end{pmatrix} \ .$$

We find $\bar{A} = \begin{pmatrix} 1 & 6 & 9 \\ 1 & 7 & 12 \\ 1 & 8 & 16 \end{pmatrix}$ and the matrix relations

$$\begin{pmatrix} 0 & 1 & 0 \\ -24 & 7 & 2 \\ 0 & -12 & 14 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ 6 & 7 & 8 \\ 9 & 12 & 16 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 6 & 7 & 8 \\ 9 & 12 & 16 \end{pmatrix}\begin{pmatrix} 6 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 8 \end{pmatrix} \ .$$

5. K-condition and Associated System

Start with U, a unitary matrix with $|U_{i0}| > 0$, $0 \le i \le d$.

Make the first column to consist of all 1's as follows. Let

$$\delta = \begin{pmatrix} U_{00} & & \\ & \ddots & \\ & & U_{d0} \end{pmatrix}$$

the diagonal matrix with diagonal entries the first column of U. D can be any diagonal matrix with positive diagonal entries and $D_{00} = 1$. The initial probabilities are given by the diagonal matrix

$$\mathrm{p} = \delta^*\delta = \begin{pmatrix} |U_{00}|^2 & & \\ & \ddots & \\ & & |U_{d0}|^2 \end{pmatrix} = \begin{pmatrix} p_0 & & \\ & \ddots & \\ & & p_d \end{pmatrix}$$

with $p_i > 0$, $\operatorname{tr} \mathrm{p} = 1$.

Remark 5.1. We consider the values p_i as probabilities corresponding to a multinomial process. Namely, a succession of independent trials each having one of the same d possible outcomes, with p_0 the probability of none of those outcomes occurring and p_i the probability of outcome i, $1 \le i \le d$.

The *generating matrix* A is defined by

$$A = \delta^{-1}\, U \sqrt{D}\ .$$

The essential property satisfied by A is

Definition 5.2. We say that A satisfies the K*-condition* if there exists a positive diagonal probability matrix p and a positive diagonal matrix D such that

$$A^*\mathrm{p}A = D\ .$$

with $A_{i0} = 1$, $0 \le i \le d$.

Remark 5.3. Note that this says that the columns of A are orthogonal with respect to the weights p_i and squared norms given by D_{ii}. *A fortiori* $A^{-1} = D^{-1}A^*\mathrm{p}$.

Let's verify the condition for our construction.

Proposition 5.4. *$A = \delta^{-1}\, U \sqrt{D}$, as defined above, satisfies the K-condition.*

Proof. We have

$$\begin{aligned} A^*\mathrm{p}A &= \sqrt{D}U^*(\delta^{-1})^*\delta^*\delta\delta^{-1}U\sqrt{D} \\ &= \sqrt{D}U^*U\sqrt{D} = D \end{aligned}$$

as required. □

Note that the K-condition implies that

$$\sqrt{\mathrm{p}}\, A \frac{1}{\sqrt{D}}$$

is unitary.

Some contexts.

(1) *Gaussian quadrature.* Let $\{\phi_0, \ldots, \phi_n\}$ be an orthogonal polynomial sequence with positive weight function on a finite interval I of the real line. For Gaussian quadrature,

$$\frac{1}{|\mathrm{I}|}\int_{\mathrm{I}} f \approx \sum_k w_k f(x_k)$$

with x_k the zeros of ϕ_n and appropriate weights w_k. Let

$$A_{ij} = \phi_{i-1}(x_j)$$

with indices running from 1 to n. Then, with Γ the diagonal matrix of squared norms, $\Gamma_{ii} = \|\phi_i\|^2$, $0 \le i < n$,we have

$$AWA^* = \Gamma$$

where W is the diagonal matrix with $W_{kk} = w_k$, $1 \le k \le n$. That is, A^* satisfies the K-condition.

(2) *Association schemes.* Given an association scheme with adjacency matrices A_i, the P and Q matrices correspond to the decomposition of the algebra generated by the A_i into an orthogonal direct sum, the entries P_{ij} being the corresponding eigenvalues. A basic result is the relation

$$P^* D_\mu P = v\, D_v$$

where D_μ is the diagonal matrix of multiplicities and D_v the diagonal matrix of valencies of the scheme. This plays an essential rôle in the work of Delsarte, Bannai, and generally in this area.

5.1. Matrices for multivariate Krawtchouk systems. For any degree N, the K-condition implies

$$\overline{A^*}\bar{\mathrm{p}}\bar{A} = \bar{D}\ .$$

Application of the Transpose Lemma

$$B\overline{A^*} = \bar{A}^* B$$

with B the special multinomial diagonal matrix yields

$$\bar{A}^*\, B\bar{\mathrm{p}}\, \bar{A} = B\bar{D}\ .$$

Definition 5.5. The *Krawtchouk matrix* Φ is defined as

$$\Phi = \bar{A}^*$$

where A is a matrix satisfying the K-condition.

Thus,

Proposition 5.6. *For A satisfying the K-condition, the Krawtchouk matrix $\Phi = \bar{A}^*$ satisfies the orthogonality relation*

$$\Phi\, B\bar{\mathrm{p}}\, \Phi^* = B\bar{D}\ .$$

The entries of Φ are the values of the **multivariate Krawtchouk polynomials** thus determined.

The rows of Φ are comprised of the values of the corresponding Krawtchouk polynomials. The relationship above indicates that these are orthogonal with respect to the associated multinomial distribution. $B\bar{D}$ is the diagonal matrix of squared norms according to the orthogonality of the Krawtchouk polynomials.

Note that the unitarity of $U = \sqrt{\mathrm{p}}\, A \dfrac{1}{\sqrt{D}}$ entails $UU^* = I$ as well. We have

Proposition 5.7. *The Krawtchouk matrix Φ satisfies dual orthogonality relations*

$$\Phi^*(B\bar{D})^{-1}\Phi = (B\bar{\mathrm{p}})^{-1} \ .$$

Proof. Rewrite the relation in Proposition 5.6 as

$$\Phi\, B\bar{\mathrm{p}}\, \Phi^*(B\bar{D})^{-1} = I \ .$$

This says $\Phi\, B\bar{\mathrm{p}}$ and $\Phi^*(B\bar{D})^{-1}$ are mutual inverses. Reversing the order gives the dual form. □

Example 5.8. Start with the orthogonal matrix

$$U = \begin{pmatrix} \sqrt{q} & \sqrt{p} \\ \sqrt{p} & -\sqrt{q} \end{pmatrix} \ .$$

Factoring out the squares from the first column we have

$$\mathrm{p} = \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} 1 & p \\ 1 & -q \end{pmatrix} \ .$$

with

$$A^*\mathrm{p}A = \begin{pmatrix} 1 & 0 \\ 0 & pq \end{pmatrix} = D \ .$$

Take $N = 4$.
We have the Krawtchouk matrix $\Phi = \bar{A}^* =$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4p & -q+3p & -2q+2p & -3q+p & -4q \\ 6p^2 & -3pq+3p^2 & q^2-4pq+p^2 & 3q^2-3pq & 6q^2 \\ 4p^3 & -3p^2q+p^3 & 2pq^2-2p^2q & -q^3+3pq^2 & -4q^3 \\ p^4 & -p^3q & p^2q^2 & -pq^3 & q^4 \end{pmatrix} \ .$$

p becomes the induced matrix

$$\bar{\mathrm{p}} = \begin{pmatrix} q^4 & 0 & 0 & 0 & 0 \\ 0 & q^3p & 0 & 0 & 0 \\ 0 & 0 & q^2p^2 & 0 & 0 \\ 0 & 0 & 0 & qp^3 & 0 \\ 0 & 0 & 0 & 0 & p^4 \end{pmatrix} \ .$$

and the binomial coefficient matrix $B = \mathrm{diag}(1, 4, 6, 4, 1)$.

Example 5.9. For an example in two variables, start with

$$U = \begin{pmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} \end{pmatrix} .$$

Taking D to be the identity, we have

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 1 & -2 \end{pmatrix} , \qquad \mathrm{p} = \begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/6 \end{pmatrix} .$$

The level two induced matrix

$$\Phi^{(2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 0 & 2 & -2 & 0 & 2 \\ 2 & 1 & -1 & 0 & -2 & -4 \\ 1 & -1 & 1 & 1 & -1 & 1 \\ 2 & -1 & -1 & 0 & 2 & -4 \\ 1 & 0 & -2 & 0 & 0 & 4 \end{pmatrix}$$

indicating the level explicitly.

Example 5.10. (An example for three variables) Here we illustrate a special property of reflections. Start with the vector $\mathbf{v}^T = (1, -1, -1, -1)$. Form the rank-one projection, $V = \mathbf{v}\mathbf{v}^T/\mathbf{v}^T\mathbf{v}$, and the corresponding reflection $U = 2V - I$:

$$U = \begin{pmatrix} -1/2 & -1/2 & -1/2 & -1/2 \\ -1/2 & -1/2 & 1/2 & 1/2 \\ -1/2 & 1/2 & -1/2 & 1/2 \\ -1/2 & 1/2 & 1/2 & -1/2 \end{pmatrix} .$$

Rescale so that the first column consists of all 1's to get

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

with the uniform distribution $p_i = 1/4$, and $D = I$. We find

$$\Phi^{(2)} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & 0 & 0 & 2 & 0 & 0 & -2 & -2 & -2 \\ 2 & 0 & 2 & 0 & -2 & 0 & -2 & 2 & 0 & -2 \\ 2 & 0 & 0 & 2 & -2 & -2 & 0 & -2 & 0 & 2 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 2 & 0 & 0 & -2 & -2 & 2 & 0 & -2 & 0 & 2 \\ 2 & 0 & -2 & 0 & -2 & 0 & 2 & 2 & 0 & -2 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\ 2 & -2 & 0 & 0 & 2 & 0 & 0 & -2 & 2 & -2 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix}$$

With $A^2 = 4I$, we have, in addition to the orthogonality relation, that $(\Phi^{(2)})^2 = 16I$.

5.2. Quantum variables and recurrence formulas. We resume from §4. Let A satisfy the K-condition. Form Λ_j from A as in the Columns Theorem. Define, for each j,

$$X_j = A^{-1}\Lambda_j A\ .$$

Observe that from the K-condition we have

$$\begin{aligned} A^{-1}\Lambda_j A &= D^{-1}A^*\delta^*\delta\Lambda_j\delta^{-1}U\sqrt{D} \\ &= D^{-1}\sqrt{D}U^*(\delta^{-1})^*\delta^*\delta\Lambda_j\delta^{-1}U\sqrt{D} \\ &= \frac{1}{\sqrt{D}}\,U^*\Lambda_j U\sqrt{D}\ . \end{aligned}$$

Thus,

Proposition 5.11. *If D equals the identity in the K-condition for A, we have*

$$X_j = A^{-1}\Lambda_j A = U^*\Lambda_j U$$

that is, conjugation by A is unitary equivalence. Thus, the X_j are quantum observables in the real case, and quantum variables generally.

Referring to equation (4.1), we have, for each j, $0 \le j \le d$,

$$\Gamma(X_j)^*\Phi = \Phi\Gamma(\Lambda_j)^*\ .$$

The left hand side induces combinations of the rows of Φ while the right hand side multiplies by diagonal elements of $\Gamma(\Lambda_j)^*$. Now Corollary 3.2 tells us that these are (complex conjugates) of the columns from $\bar{A}$, equivalently, rows of Φ. These are the rows with labels 1 through d thus corresponding to the polynomials x_j, $1 \le j \le d$. Thus, we interpret the above equation as the relation

$$(\mathrm{Rec})\,\Phi = \Phi\,(\mathrm{Spec})$$

that is, these are recurrence relations for the multivariate Krawtchouk polynomials.

In this next example, we keep the variable v and see that our procedure gives multiplication by higher-order polynomials thus yielding more complex recurrence formulas.

Example 5.12. Start with the orthogonal matrix $U = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$.

Factoring out the squares from the first column we have

$$\mathrm{p} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} .$$

satisfying $A^*\mathrm{p}A = I$. We have the Krawtchouk matrix in degree 4

$$\Phi = \bar{A}^* = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix} .$$

The entries of p become $\bar{\mathrm{p}} = \dfrac{1}{16} I_5$ with the binomial coefficient matrix $B = \mathrm{diag}(1, 4, 6, 4, 1)$.

Take the second column of A, recalling that our indexing starts with 0, and form the diagonal matrix

$$\Lambda_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The corresponding observable is

$$X_1 = A^{-1}\Lambda_1 A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

Let $\Lambda = I + v\Lambda_1$ and $X = I + v\,X_1$. Then in degree 4,

$$\bar{\Lambda} = \mathrm{diag}((1+v)^4, (1+v)^3(1-v), (1+v)^2(1-v)^2, (1+v)(1-v)^3, (1-v)^4),$$

and

$$\bar{X} = \begin{pmatrix} 1 & 4v & 6v^2 & 4v^3 & v^4 \\ v & 1+3v^2 & 3v+3v^3 & 3v^2+v^4 & v^3 \\ v^2 & 2v+2v^3 & 1+4v^2+v^4 & 2v+2v^3 & v^2 \\ v^3 & 3v^2+v^4 & 3v+3v^3 & 1+3v^2 & v \\ v^4 & 4v^3 & 6v^2 & 4v & 1 \end{pmatrix} .$$

Now we have the spectrum via the coefficient of v in $\bar{\Lambda}$

$$\mathrm{Spec} = \mathrm{diag}(4, 2, 0, -2, -4)$$

which is the same as the row with label 1 in Φ. The coefficient of v in the transpose of $\bar{X}$ give the recurrence coefficients

$$\mathrm{Rec} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 4 & 0 & 2 & 0 & 0 \\ 0 & 3 & 0 & 3 & 0 \\ 0 & 0 & 2 & 0 & 4 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

satisfying the relation

$$(\mathrm{Rec})\,\Phi = \Phi\,(\mathrm{Spec})$$

which is essentially the recurrence relation for the corresponding Krawtchouk polynomials. Coefficients of higher powers of v thus correspond to higher-order recurrence relations corresponding to multiplication by higher order Krawtchouk polynomials. For example, the coefficient of v^2 yields the relations

$$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 3 & 0 & 3 & 0 \\ 6 & 0 & 4 & 0 & 6 \\ 0 & 3 & 0 & 3 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 6 \end{pmatrix}$$

etc.

Example 5.13. Continuing with Example 5.9,

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & 1 & -2 \end{pmatrix}, \qquad \mathrm{p} = \begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/6 \end{pmatrix}$$

and D the identity. The level two Krawtchouk matrix

$$\Phi = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 0 & 2 & -2 & 0 & 2 \\ 2 & 1 & -1 & 0 & -2 & -4 \\ 1 & -1 & 1 & 1 & -1 & 1 \\ 2 & -1 & -1 & 0 & 2 & -4 \\ 1 & 0 & -2 & 0 & 0 & 4 \end{pmatrix}.$$

We have the (pre)spectral matrices

$$\Lambda_1 = \mathrm{diag}(1,-1,1) \qquad \text{and} \qquad \Lambda_2 = \mathrm{diag}(1,0,-2)$$

with Λ_0 the 3×3 identity. Conjugating by A yields

$$X_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Cranking up to degree 2 we have

$$\Gamma(X_1)^* = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \Gamma(X_2)^* = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 2 & 1 & -1 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 2 & -1 & 2 \\ 0 & 0 & 1 & 0 & 1 & -2 \end{pmatrix}$$

with spectra

$$\Gamma(\Lambda_1) = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \Gamma(\Lambda_2) = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & -4 \end{pmatrix}$$

with no adjoints necessary in the real case.

6. Illustrative Cases

6.1. Reflections. Given a vector $\mathbf{v}$, form the reflection

$$U = R_{\mathbf{v}} = 2(\mathbf{v}\mathbf{v}^*/\mathbf{v}^*\mathbf{v}) - I$$

fixing $\mathbf{v}$. This is both self-adjoint and unitary, $U^2 = I$. The Krawtchouk matrix Φ will have interesting special properties in this case.

Proposition 6.1. *Let U be a unitary reflection and let A be the corresponding generating matrix for the KG-system:*

$$A = \delta^{-1} U \sqrt{D}$$

where δ is the diagonal matrix with diagonal elements from the first column of U. Let Φ be the Krawtchouk matrix for a given degree. Then:

1. Involutive property: $\left(\overline{\delta^* D^{-1/2}}\,\Phi\right)^2 = I$.
2. Self-adjointness: $\Phi B \bar{\delta}^* \overline{D^{1/2}}$ *is self-adjoint.*

Proof. For #1,

$$U^2 = \delta A D^{-1/2} \delta A D^{-1/2} = I$$

Now multiply by δ^{-1} on the left and multiply back by δ on the right to get

$$(A\delta D^{-1/2})^2 = I \ .$$

Now bar and star to get

$$(\overline{\delta^* D^{-1/2}}\bar{A}^*)^2 = I$$

and replacing $\bar{A}^*$ with Φ yields the result.

For #2, start with

$$\delta A D^{-1/2} = D^{-1/2} A^* \delta^* \ .$$

Rearrange to

$$\delta D^{1/2} A = A^* \delta^* D^{1/2} \ .$$

Now bar to get
$$\bar\delta\,\overline{D^{1/2}}\bar A = \overline{A^*}\bar\delta^*\overline{D^{1/2}}\ .$$
In terms of Φ, this is
$$\bar\delta\,\overline{D^{1/2}}\Phi^* = B^{-1}\Phi B\bar\delta^*\overline{D^{1/2}}\ .$$
Multiplying through by B on the left yields
$$\bar\delta\,\overline{D^{1/2}}B\Phi^* = \Phi B\bar\delta^*\overline{D^{1/2}}$$
as required. □

Example 6.2. Here's an example which illustrates the various quantities involved. Starting with $\mathbf{v} = (1, 2i)^T$, form the reflection
$$U = R_{\mathbf{v}} = \begin{pmatrix} -\frac{3}{5} & -\frac{4i}{5} \\ \frac{4i}{5} & \frac{3}{5} \end{pmatrix}\ .$$
Factoring out $\delta = \begin{pmatrix} -\frac{3}{5} & 0 \\ 0 & \frac{4i}{5} \end{pmatrix}$, we take $D = \begin{pmatrix} 1 & 0 \\ 0 & 36 \end{pmatrix}$ so that
$$A = \delta^{-1}U\sqrt{D} = \begin{pmatrix} 1 & 8i \\ 1 & -\frac{9i}{2} \end{pmatrix} \qquad \text{and} \qquad \mathrm{p} = \begin{pmatrix} \frac{9}{25} & 0 \\ 0 & \frac{16}{25} \end{pmatrix}\ .$$
In degree 3,
$$\Phi = \begin{pmatrix} 1 & 1 & 1 & 1 \\ -24i & -\frac{23i}{2} & i & \frac{27i}{2} \\ -192 & 8 & \frac{207}{4} & -\frac{243}{4} \\ 512i & -288i & 162i & -\frac{729i}{8} \end{pmatrix}$$
with $B = \mathrm{diag}(1, 3, 3, 1)$.

We have the involution
$$\overline{\delta^* D^{-1/2}}\,\Phi = \begin{pmatrix} -\frac{27}{125} & -\frac{27}{125} & -\frac{27}{125} & -\frac{27}{125} \\ -\frac{144}{125} & -\frac{69}{125} & \frac{6}{125} & \frac{81}{125} \\ -\frac{256}{125} & \frac{32}{375} & \frac{69}{125} & -\frac{81}{125} \\ -\frac{4096}{3375} & \frac{256}{375} & -\frac{48}{125} & \frac{27}{125} \end{pmatrix}$$
and the self-adjoint matrix
$$\Phi B\bar\delta^*\overline{D^{1/2}} = \begin{pmatrix} -\frac{27}{125} & -\frac{648i}{125} & \frac{5184}{125} & \frac{13824i}{125} \\ \frac{648i}{125} & -\frac{7452}{125} & \frac{5184i}{125} & -\frac{186624}{125} \\ \frac{5184}{125} & -\frac{5184i}{125} & \frac{268272}{125} & -\frac{839808i}{125} \\ -\frac{13824i}{125} & -\frac{186624}{125} & \frac{839808i}{125} & \frac{1259712}{125} \end{pmatrix}\ .$$

6.2. Symmetric binomial. Let us look at the binomial case with equal probabilities. This is the basic case for the original version of Krawtchouk's polynomials.

We start with the orthogonal matrix $U = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$ with

$$\mathrm{p} = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \quad \text{and} \quad A = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} .$$

satisfying $A^*\mathrm{p}A = I$.

Recalling Example 5.12, consider $N = 4$ from which we will see the pattern for general N. We have the recurrence relations

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 4 & 0 & 2 & 0 & 0 \\ 0 & 3 & 0 & 3 & 0 \\ 0 & 0 & 2 & 0 & 4 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 4 & 2 & 0 & -2 & -4 \\ 6 & 0 & -2 & 0 & 6 \\ 4 & -2 & 0 & 2 & -4 \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & -4 \end{pmatrix} .$$

With j the column index, the spectrum has the form $x = N - 2j$. Denoting by K_n the rows of the Krawtchouk matrix, i.e., these are the Krawtchouk polynomials when expressed as functions of x, we read off the recurrence relations

$$(N - (n-1))K_{n-1} + (n+1)K_{n+1} = xK_n$$

with initial conditions $K_0 = 1$, $K_1 = x$. The polynomials may be expressed in terms of either x or j. For example

$$\begin{aligned} K_1 &= x \ , & K_1 &= N - 2j \\ K_2 &= \frac{1}{2}(x^2 - N) \ , & K_2 &= \frac{1}{2}(4j^2 - 4jN + N^2 - N) \\ K_3 &= \frac{1}{6}(x^3 - 3xN + 2x) \ , & & \ldots \end{aligned}$$

Recalling $\bar{\Lambda}$ from Example 5.12 we see the form for the generating function

$$(1+v)^{N-j}(1-v)^j = \sum_n v^n K_n(j)$$

via the Columns Theorem.

In this context U is a reflection, with $\mathrm{p} = (1/2)I$, $D = I$. We have, specializing from §6.1,

$$\Phi^2 = 2^N\, I \qquad \text{and} \qquad (\Phi B)^* = \Phi B$$

involutive and symmetry properties respectively.

7. Conclusion

Here we have presented the approach to multivariate Krawtchouk polynomials using matrices, working directly with the values they take. With this approach the algebraic structures are clearly seen.

In KG-Systems II, we present the analytical side. In particular, the KG-systems as Bernoulli systems is presented showing how these are discrete quantum systems. The Fock space structure and observables are discussed in detail.

We conclude with the observation that there are many unanswered questions involving Krawtchouk matrices, for example, the behavior of the largest eigenvalue for the symmetric Krawtchouk matrices in the classical case is an interesting open problem [3].

Remark 7.1. Symbolic computations have been done using IPython. Some IPython notebooks for computations and examples are available at:

`http://ziglilucien.github.io/NOTEBOOKS`

which will be updated as that project develops.

Finally, as these are finite quantum systems, possible connections with quantum computation are intriguing.

8. Appendix

Theorem 8.1. (Basic properties of the Γ-map for the symmetric representation) *The first two properties show that Γ is a linear map. The third shows that it is a Lie homomorphism.*

1. *For scalar λ, $\Gamma(\lambda X) = \lambda\Gamma(X)$.*
2. *Additivity holds: $\Gamma(X+Y) = \Gamma(X) + \Gamma(Y)$.*
3. *With $[X,Y] = XY - YX$ denoting the commutator of X and Y, we have*

$$\Gamma([X,Y]) = [\Gamma(X), \Gamma(Y)] \ .$$

Proof. For Property #1 start from the definition:

$$\overline{e^{t\lambda X}} = e^{\lambda t\Gamma(X)} = e^{t\Gamma(\lambda X)}$$

and differentiating with respect to t at 0 gives #1.

For #2,

$$\overline{e^{t(X+Y)}} = e^{t\Gamma(X+Y)}$$

by definition. Now we use multiplicativity and the Trotter product formula as follows:

$$\begin{aligned}
\overline{e^{t(X+Y)}} &= \lim_{n\to\infty} \overline{\left(e^{(t/n)X}e^{(t/n)Y}\right)^n} \\
&= \lim_{n\to\infty} \left(\overline{e^{(t/n)X}}\ \overline{e^{(t/n)Y}}\right)^n \\
&= \lim_{n\to\infty} \left(e^{(t/n)\Gamma(X)}\ e^{(t/n)\Gamma(Y)}\right)^n \\
&= e^{t(\Gamma(X)+\Gamma(Y))}
\end{aligned}$$

and differentiating with respect to t at 0 yields the result.

For #3 we use the adjoint representation, with $(\operatorname{ad} X)Y = [X, Y]$,

$$e^{tX} Y e^{-tX} = e^{t \operatorname{ad} X} Y = Y + t[X, Y] + \frac{t^2}{2} [X, [X, Y]] + \cdots + \frac{t^n}{n!} (\operatorname{ad} X)^n Y + \cdots$$

Write this as

$$e^{tX} Y e^{-tX} = Y + t[X, Y] + \mathcal{O}(t^2)$$

Then

$$\overline{e^{tX} e^{sY} e^{-tX}} = \overline{e^{s(Y + t[X,Y] + \mathcal{O}(t^2))}}$$

By multiplicativity and linearity we have

$$e^{t\Gamma(X)} e^{s\Gamma(Y)} e^{-t\Gamma(X)} = e^{s\Gamma(Y) + st\Gamma([X,Y]) + s\mathcal{O}(t^2)}$$

Now, differentiating with respect to s at 0 yields

$$e^{t\Gamma(X)} \Gamma(Y) e^{-t\Gamma(X)} = \Gamma(Y) + t\Gamma([X, Y]) + \mathcal{O}(t^2)$$

Differentiating with respect to t at 0 finishes the proof. □

Acknowledgment. The author would like to thank the organizers of the 33rd Quantum Probability conference, Luminy, 2012, where a portion of this work was presented.

References

1. Bose, N. K.: *Digital Filters: Theory and Applications.* North-Holland, 1985.
2. Diaconis, Persi and Griffiths, Robert: An introduction to multivariate Krawtchouk polynomials and their applications. *J. Statist. Plann. Inference*, 154:39–53, 2014.
3. Feinsilver, Philip and Fitzgerald, Robert: The spectrum of symmetric Krawtchouk matrices. *Lin. Alg. & Appl.*, 235:121–139, 1996.
4. Feinsilver, Philip and Kocik, Jerzy : Krawtchouk matrices from classical and quantum random walks. In *Algebraic methods in statistics and probability (Notre Dame, IN, 2000)*, volume 287 of *Contemp. Math.*, pages 83–96. Amer. Math. Soc., Providence, RI, 2001.
5. Feinsilver, Philip and Schott, René: *Algebraic Structures and Operator Calculus. Vol. III*, volume 347 of *Mathematics and its Applications.* Kluwer Academic Publishers Group, Dordrecht, 1996. Representations of Lie groups.
6. Feinsilver, Ph. and Schott, R.: On Krawtchouk Transforms. *Intelligent Computer Mathematics*, proceedings 10th Intl. Conf. AISC 2010, LNAI 6167:64–75, 2010.
7. Griffiths, R. C.: Orthogonal polynomials on the multinomial distribution. *Austral. J. Statist.*, 13:27–35, 1971.
8. Griffiths, R. C.: A characterization of the multinomial distribution. *Austral. J. Statist.*, 16:53–56, 1974.
9. Griffiths, Robert: Multivariate Krawtchouk polynomials and composition birth and death processes. *Symmetry*, 8(5):Art. 33, 19, 2016.
10. Grünbaum, F. Alberto and Rahman, Mizan: On a family of 2-variable orthogonal Krawtchouk polynomials. *SIGMA Symmetry Integrability Geom. Methods Appl.*, 6:Paper 090, 12, 2010.
11. Grünbaum, F. Alberto and Rahman, Mizan: A system of multivariable Krawtchouk polynomials and a probabilistic application. *SIGMA Symmetry Integrability Geom. Methods Appl.*, 7:Paper 119, 17, 2011.
12. Kocik, Jerzy: Krawtchouk matrices, Feynman path integral and the split quaternions. In *Probability on algebraic and geometric structures (Carbondale, IL, 2014)*, volume 668 of *Contemp. Math.*, pages 131–164. Amer. Math. Soc., Providence, RI, 2016.
13. Koornwinder, Tom H.: Krawtchouk polynomials, a unification of two different group theoretic interpretations. *SIAM J. Math. Anal.*, 13(6):1011–1023, 1982.

14. Krawtchouk, M.: Sur une généralisation des polynômes d'Hermite. *Comptes Rendus*, 189:620–622, 1929.
15. Mizukawa, Hiroshi and Tanaka, Hajime: $(n+1, m+1)$-hypergeometric functions associated to character algebras. *Proc. Amer. Math. Soc.*, 132(9):2613–2618(electronic), 2004.
16. Sloane, N. J. A.: Error-correcting codes and invariant theory: new applications of a nineteenth-century technique. *Amer. Math. Monthly*, 84(2):82–107, 1977.
17. Springer, Tonny A.: Invariant Theory. *Lecture Notes in Mathematics*, 585, Springer-Verlag, 1977.

Philip Feinsilver: Department of Mathematics Southern Illinois University, Carbondale, Illinois 62901, USA
E-mail address: `phfeins@siu.edu`