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## Random unistochastic matrices

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### Abstract

An ensemble of random unistochastic (orthostochastic) matrices is defined by taking squared moduli of elements of random unitary (orthogonal) matrices distributed according to the Haar measure on  $U(N)$  (or  $O(N)$ ). An ensemble of symmetric unistochastic matrices is obtained with use of unitary symmetric matrices pertaining to the circular orthogonal ensemble. We study the distribution of complex eigenvalues of bistochastic, unistochastic and orthostochastic matrices in the complex plane. We compute averages (entropy, traces) over the ensembles of unistochastic matrices and present inequalities concerning the entropies of products of bistochastic matrices.

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### 1. Introduction

Consider a square matrix  $B$  of size  $N$  containing non-negative entries. It is called *stochastic* if each row sums to unity ( $\sum_{i=1}^N B_{ij} = 1$  for  $j = 1, \dots, N$ ) (for information about properties of such matrices consult [1, 2]). If, additionally, each of its columns sums to unity, i.e.,  $\sum_{j=1}^N B_{ij} = 1$  for  $i = 1, \dots, N$ , it is called *bistochastic* (or *doubly stochastic*).

Bistochastic matrices emerge in several physical problems. They are used in the theory of majorization [3–6], angular momentum [7], transfer problems, investigations of the Frobenius–Perron operator and in characterization of completely positive maps acting in the space of density matrices [8]. We shall denote by  $\Omega_N^S$  (respectively  $\Omega_N^B$ ) the sets of stochastic (respectively bistochastic) matrices of size  $N$ .

A matrix  $B$  is called *orthostochastic* if there exists an orthogonal matrix  $O$  such that  $B_{ij} = O_{ij}^2$  for  $i, j = 1, \dots, N$ . Analogously, a matrix  $B$  is called *unistochastic* (*unitary-stochastic*)<sup>5</sup> if there exists a unitary matrix  $U$ , such that  $B_{ij} = |U_{ij}|^2$  for  $i, j = 1, \dots, N$ .

<sup>5</sup> This notation is not unique: in some mathematical papers (e.g. [43]) unistochastic matrices are called orthostochastic.

Due to the unitarity (orthogonality) condition every unistochastic (orthostochastic) matrix is bistochastic. These four sets of non-negative matrices are related by the following inclusion:  $\Omega_N^O \subseteq \Omega_N^U \subseteq \Omega_N^B \subseteq \Omega_N^S$ , where  $\Omega_N^U$  and  $\Omega_N^O$  represent the sets of unistochastic (orthostochastic) matrices. For  $N > 2$  all three inclusions are proper [3].

Unistochastic matrices appear in the analysis of models describing the time evolution in quantum graphs [9–13] and in the description of non-unitary transformations of density matrices [14, 15]. Moreover, the theory of majorization and unistochastic matrices plays a crucial role in recent research on local manipulations with pure states entanglement [16] or in characterizing the interaction costs of non-local quantum gates [17].

In this work we analyse the structure of the set of bistochastic (unistochastic) matrices of fixed size and investigate the support of their spectra. Knowledge of any constraints for the localization of the eigenvalues of such a matrix is of direct physical importance, since the moduli of the second largest eigenvalues determine the rate of relaxation to the invariant state of the corresponding system. We define the notion of entropy of bistochastic matrices and prove certain inequalities comparing the initial and the final entropy of any probability vector subjected to a Markov chain described by an arbitrary bistochastic matrix. A related inequality concerns the entropy of the product of two bistochastic matrices.

Moreover, we define physically motivated ensembles of random unistochastic matrices and analyse their properties. As usual, the term *ensemble* denotes a pair: a space and a probability measure defined on it (for example, the *circular unitary ensemble* (CUE) represents the group  $U(N)$  of unitary matrices of size  $N$  with the Haar measure [18]). Since any unitary matrix determines a unistochastic matrix, the Haar measure on the unitary group  $U(N)$  induces uniquely the measure in the space of unistochastic matrices  $\Omega_N^U$ , which we shall denote by  $\mu_U$ . Analogously, we shall put  $\mu_O$  for the measure in  $\Omega_N^O$  induced by the Haar measure on the orthogonal group  $O(N)$ . In what follows we shall use the terms *unistochastic ensemble* (respectively *orthostochastic ensemble*) for the pair  $(\Omega_N^U, \mu_U)$  (respectively  $(\Omega_N^O, \mu_O)$ ).

We compute certain averages with respect to these ensembles. Related results were presented recently by Berkolaiko [19] and Tanner [12]. In the latter paper the author defines unitary stochastic ensembles, which have a different meaning: they consist of unitary matrices corresponding to a given unistochastic matrix.

This paper is organized as follows. In section 2 we review properties of stochastic matrices. In particular we analyse the support of spectra of random bistochastic and stochastic matrices in the unit circle. In section 3 some results concerning majorization, ordering and entropies of bistochastic matrices are presented. In particular we prove subadditivity of entropy for bistochastic matrices. Section 4 is devoted to the ensembles of orthostochastic and unistochastic matrices; we investigate the support of their spectra, compute the entropy averages, the average traces and expectation values of the moduli of subleading eigenvalues. Some open problems are listed in section 5. Analysis of certain families of unistochastic matrices and calculation of the averages with respect to the unistochastic ensemble is relegated to the appendices.

## 2. Stochastic and bistochastic matrices

### 2.1. General properties

In this section we provide a brief review of properties of stochastic and bistochastic matrices. The set of bistochastic matrices of size  $N$  can be viewed as a convex polyhedron in  $R^{N^2}$ . There exist  $N!$  permutation matrices of size  $N$ , obtained by interchanging the rows (or columns) of the identity matrix. Due to the Birkhoff theorem, any bistochastic matrix can be represented as

a linear combination of permutation matrices. In other words, the set of bistochastic matrices is the convex hull of the set of permutation matrices. By the Carathéodory theorem it is possible to use only  $N^2 - 1$  permutation matrices to obtain a given bistochastic matrix as their convex combination [3]. Farahat and Mirsky showed that in this combination it is sufficient to use  $N^2 - 2N + 2$  permutation matrices only, but this number cannot be reduced any further [20]. The dimension of the set of bistochastic matrices is  $(N - 1)^2$ . The volume of the polyhedron of bistochastic matrices was computed by Chan and Robbins [21].

Due to the Frobenius–Perron theorem any stochastic matrix has at least one eigenvalue equal to 1, and all others located at or inside the unit circle. The eigenvector corresponding to the eigenvalue 1 has all its components real and non-negative. For bistochastic matrices the corresponding eigenvector consists of  $N$  components equal to  $1/N$  and is called uniform. A stochastic matrix  $S$  is called *reducible* if it is block diagonal, or if there exists a permutation  $P$  which brings it into a block structure,

$$S' = PSP^{-1} = \begin{bmatrix} A_1 & 0 \\ C & A_2 \end{bmatrix} \quad (2.1)$$

where  $A_i$  are square matrices of size  $N_i < N$  for  $i = 1, 2$ ,  $N = N_1 + N_2$ . It is called *decomposable* if one can find two permutation matrices  $P$  and  $Q$  such that  $PSQ$  has the above form. Matrix  $S$  is *irreducible (indecomposable)* if no such matrix  $P$  (matrices  $P$  and  $Q$ ) exists (exist) [3, 22]. An irreducible stochastic matrix cannot have two linearly independent vectors with all components non-negative. Any reducible bistochastic matrix is *completely reducible* [22], i.e., the matrix  $C$  in (2.1) is equal to zero.

A stochastic matrix  $S$  is called *primitive* if there exists only one eigenvalue with modulus equal to 1. If  $S$  is primitive, then  $S^k$  is irreducible for all  $k \geq 1$  [3]. Note that the permutation matrices  $P$  with  $\text{tr } P = 0$  are irreducible, but non-primitive, since  $P^N$  equal to the identity matrix is reducible. For any primitive stochastic matrix, there exists a natural number  $k$  such that the power  $S^k$  has all entries positive. If  $B$  is a bistochastic primitive matrix then the unity implies the convergence  $\lim_{k \rightarrow \infty} B^k = B_*$ . Here  $B_*$  denotes the uniform bistochastic matrix (*van der Waerden matrix*) with all elements equal to  $1/N$ . Its spectrum consists of one eigenvalue equal to 1 and  $N - 1$  others equal to zero. The matrix  $B_*$  saturates the well known van der Waerden inequality [3] concerning the permanent of the bistochastic matrices:  $\text{per } B \geq N!/N^N$ , and hence is sometimes called the *minimal* bistochastic matrix [22, 23].

Each bistochastic matrix of size  $N$  may represent a transfer process at an oriented graph consisting of  $N$  nodes. If a graph is disjoint or consists of a Hamilton cycle (which represents a permutation of all  $N$  elements), the bistochastic matrix is not primitive, and the modulus of the subleading eigenvalue (the second largest) is equal to unity.

If matrices  $A$  and  $B$  are bistochastic, its product  $C = AB$  is also bistochastic. However, the set of bistochastic matrices does not form a group, since in general the inverse matrix  $A^{-1}$  is not bistochastic (if it exists). For any permutation matrix  $P$ , its inverse  $P^{-1} = P^T$  is bistochastic and the eigenvalues of  $P$  and  $P^{-1}$  are equal and belong to the unit circle.

## 2.2. Spectra of stochastic matrices

A stochastic matrix contains only non-negative entries and due to the Frobenius–Perron theorem its largest eigenvalue is real. This leading eigenvalue is equal to unity, since its spectral radius is bounded by the largest and the smallest sum of its rows, all of which are equal to 1. In the simplest case of permutation matrices the spectrum consists of some roots of unity. The eigenvalues of permutation matrices consisting of only one cycle of length  $k$  are exactly the  $k$ th roots of unity.

Upper bounds for the size of the other eigenvalues are given in [24]. Let  $M$  denote the largest element of a stochastic matrix and  $m$  the smallest. Then the radius  $r_2$  of a subleading eigenvalue satisfies

$$r_2 \leq \frac{M - m}{M + m}. \quad (2.2)$$

From this bound it follows that all subleading eigenvalues of the van der Waerden uniform matrix  $B_*$  vanish. Another simple bound of this kind for a matrix of size  $N$  reads

$$r_2 \leq \min\{NM - 1, 1 - Nm\}. \quad (2.3)$$

For any stochastic matrix, the characteristic polynomial is real, so we may expect a clustering of the eigenvalues of random stochastic matrices at the real line. This issue is related to the result of Kac, who showed that the number of real roots of a polynomial of order  $N$  with random real coefficients scales asymptotically like  $\ln N$  [25]. The spectrum of a stochastic matrix is symmetric with respect to the real axis. Thus for  $N = 2$  all eigenvalues are real and the support of the spectrum of the set of stochastic matrices reduces to the interval  $[-1, 1]$ .

Let  $Z_k$  denote a regular polygon (with its interior) centred at 0 with one of its  $k$  corners at 1. The corners are the roots of unity of order  $k$ . Let  $\bar{E}_N$  represent the convex hull of  $E_N = \bigcup_{k=2}^N Z_k$ , or in other words, the polygon constructed of all  $k$ th roots of unity, with  $k = 2, \dots, N$ . It is not difficult to show that the support  $\Sigma_n^S$  of the spectrum of a stochastic matrix of order  $N$  is contained in  $\bar{E}_n$ , see e.g. a concise proof of Schaefer [24], p 15 (originally formulated for bistochastic matrices). The corners of the polygon  $\bar{E}_N$  represent eigenvalues of non-trivial permutation matrices of size  $k$ . For  $N = 3$  this polygon becomes a deltoid (dotted lines in figure 1(a)), while for  $N = 4$  it becomes a non-regular hexagon. However, this set is larger than required, as shown by Dimitriev and Dynkin [26] for small  $N$  and later generalized and improved by Karpelevich [27] for an arbitrary matrix size; the support  $\Sigma_N^S$  of the spectrum of stochastic matrices forms, in general, a set which is not convex. For a recent simplified proof of these statements, consult papers by Djoković [28] and Ito [29]. For instance, the support  $\Sigma_3^S$  consists of a horizontal interval and the equilateral triangle (see figure 1(a)), while for  $\Sigma_4^S$  four sides of the hexagon should be replaced by the arcs, interpolating between the roots of the unity, and given by the solutions  $\lambda = |\lambda(t)| e^{i\phi(t)}$  with  $t \in [0, 1]$  of

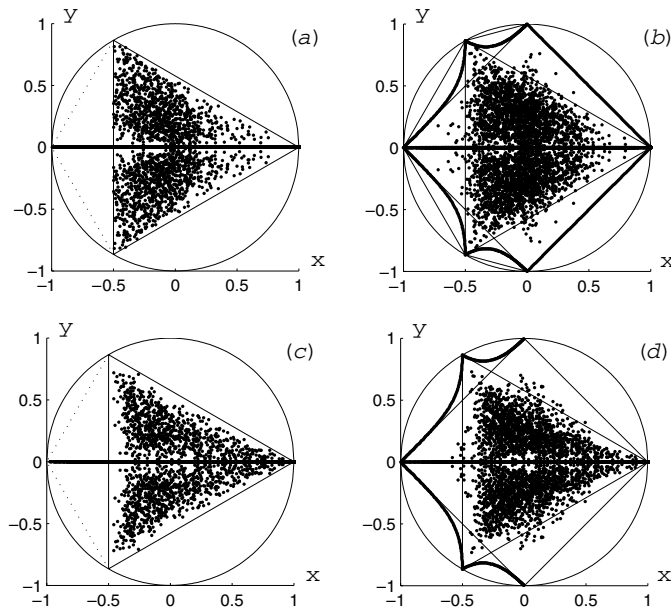
$$\lambda^3 + \lambda^2 + \lambda + t = 0 \quad \text{for which} \quad |\phi(t)| \in [\pi/2, 2\pi/3]$$

and

$$\lambda^4 - 2t\lambda^2 + (1 - t)^3\lambda + t^2 = 0 \quad \text{for which} \quad |\phi(t)| \in [2\pi/3, \pi]. \quad (2.4)$$

### 2.3. Spectra of bistochastic matrices

The *spectral gap* of a stochastic matrix is defined as  $1 - r_2$ , where  $r_2$  denotes the modulus of the subleading eigenvalue [19] (note that in [12] the gap is defined as  $-\ln r_2$ ). This quantity is relevant for several applications since it determines the speed of the relaxation to the equilibrium of the dynamical system for which  $B$  is the transition matrix. Analysing the spectrum of a bistochastic matrix, it is also interesting to study the distance of the closest eigenvalue to unity. Since for any bistochastic matrix, 1 is its simple eigenvalue if and only if the matrix is irreducible, some information on the spectrum may be obtained by introducing



**Figure 1.** Eigenvalues of 3000 random stochastic matrices of size (a)  $N = 3$ , (b)  $N = 4$ . Panels (c) and (d) show the spectra of bistoochastic matrices of sizes 3 and 4. Thick solid lines in (d) represent the bounds (2.4) of Karpelevich.

a measure of irreducibility. Such a strategy was pursued by Fiedler [30], who defined for any bistoochastic matrix  $B$  the following quantities

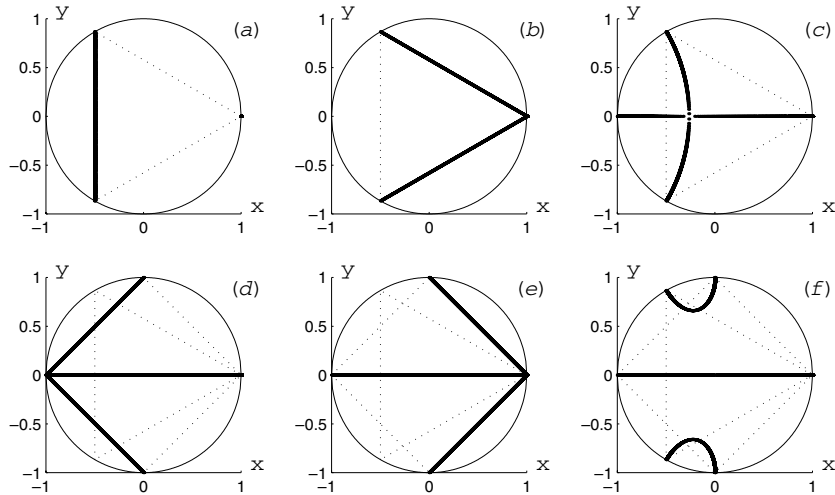
$$\mu(B) := \min_A \sum_{i \in A} \sum_{j \in \bar{A}} B_{ij} \quad \text{and} \quad \nu(B) := \min_A \sum_{i \in A} \sum_{j \in \bar{A}} \frac{B_{ij}}{n(N-n)} \tag{2.5}$$

where  $A$  is a proper subset of indices  $I = \{1, 2, \dots, N\}$  containing  $n$  elements,  $1 \leq n < N$ , and  $\bar{A}$  denotes its complement such that  $A \cup \bar{A} = I$ . Observe that  $\mu$  measures the minimal total weight of the ‘non-diagonal’ block of the matrix, which equals zero for reducible matrices, while  $\nu$  is averaged over the number of  $n(N - n)$  elements, which form such a block. Fiedler [30] used these quantities to establish the bounds for the subleading eigenvalue  $\lambda_2$

$$|1 - \lambda_2| \geq 2\mu(B) \left(1 - \cos \frac{\pi}{N}\right) \quad \text{and} \quad |1 - \lambda_2| \geq 2\nu(B). \tag{2.6}$$

Since  $\Omega_N^B \subseteq \Omega_N^S$ , the supports of the spectra fulfil  $\Sigma_N^B \subseteq \Sigma_N^S$ . Moreover, our numerical analysis suggests that for  $N \geq 4$  this inclusion is proper. In fact, they do not contradict an appealing conjecture [2] that the support  $\Sigma_N^B$  of the spectra of bistoochastic matrices is equal to the set theoretical sum  $E_N$  of regular  $k$ -polygons  $Z_k$  ( $k = 2, \dots, N$ ), whose corners are the consecutive roots of unity. Numerical results obtained for random matrices chosen according to the uniform measure in the  $(N - 1)^2$ -dimensional space of bistoochastic matrices are shown in figures 1(c) and (d).

It is not difficult to show that these polygons are indeed contained in the set  $\Sigma_N^B$ , i.e., for each  $\lambda \in \bigcup_{k=2}^N Z_k$  there exists an  $N \times N$  bistoochastic matrix  $B$  such that  $\lambda$  belongs to its spectrum,  $\text{Sp}(B)$ . First note that the support  $\Sigma_{N-1}^B$  is included in  $\Sigma_N^B$ . Hence, it is enough to show that  $Z_N \subset \Sigma_N^B$ . Let us start from the following simple observation: if  $A, B \in \Omega_N^B$  commute, then the corresponding eigenspaces are equal, and if  $\lambda \in \text{Sp}(A)$ ,  $\mu \in \text{Sp}(B)$  are the corresponding eigenvalues, then  $x\lambda + (1 - x)\mu \in \text{Sp}(xA + (1 - x)B)$  for each  $x \in [0, 1]$ .



**Figure 2.** Eigenvalues of families of bistochastic matrices, which produce the boundary of the set  $\Sigma_N^B$ . They are constructed of linear combinations,  $xP_a + (1-x)P_b$ , of permutation matrices of size  $N = 3$ : (a)  $(P_{(123)}$  and  $P_{(132)}$ ), (b)  $(P_{(123)}$  and  $I_3$ ), (c)  $(P_{(12)(3)}$  and  $I_2$ ) and of size  $N = 4$ : (d)  $(P_{(1432)}$  and  $P_{(13)(24)}$ ), (e)  $(P_{(1432)}$  and  $I_4$ ) and (f)  $(P_{(1342)}$  and  $P_{(132)(4)}$ ). Panels (a), (b), (d), and (f) show spectra of combinations of commuting and (c) and (e) of non-commuting matrices.

In what follows  $P_{(i_1^1 \dots i_{k_1}^1) \dots (i_1^m \dots i_{k_m}^m)}$  will denote the matrix, which corresponds to the permutation consisting of  $m$  cycles:  $(i_1^1 \rightarrow \dots \rightarrow i_{k_1}^1 \rightarrow i_1^1), \dots, (i_1^m \rightarrow \dots \rightarrow i_{k_m}^m \rightarrow i_1^m)$ , where  $k_1 + \dots + k_m = N$ . Let  $w_N$  be a vector whose coordinates are the consecutive  $N$ th roots of the unity, i.e.,  $w_N = (1, \exp(2\pi i/N), \dots, \exp(2\pi i(N-1)/N))$ . Let  $k = 0, \dots, N-1$ . Then matrices  $P_{(1 \dots N)}^{N-k}$  and  $P_{(1 \dots N)}^{N-(k+1)}$  commute, and  $P_{(1 \dots N)}^{N-k} w_N = \exp(2\pi k i/N) w_N$ ,  $P_{(1 \dots N)}^{N-(k+1)} w_N = \exp(2\pi(k+1)i/N) w_N$ . Hence the edges joining the complex numbers  $\exp(2\pi k i/N)$  and  $\exp(2\pi(k+1)i/N)$  for  $k = 0, \dots, N-1$  are contained in  $\Sigma_N^B$ , and so the whole boundary of the polygon  $Z_N$ . Furthermore, taking linear combinations of a bistochastic matrix with an eigenvalue at the edge of the polygon  $Z_N$  and the identity matrix  $\mathbb{I}_N$ , we may generate lines in  $\Sigma_N^B$  joining this boundary with point 1. It follows therefore that the entire inner part of each polygon constitutes a part of the support of the spectrum of the set of bistochastic matrices.

Let us now analyse in detail the case  $N = 3$ . Recall that  $P_{(123)}$  denotes the  $3 \times 3$  matrix representing the permutation  $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$ . Its third power is equal to identity,  $P_{(123)}^3 = P_{(1)(2)(3)} = \mathbb{I}_3$ , while  $P_{(123)}^2 = P_{(123)}^{-1} = P_{(132)}$ . Two edges of the equilateral triangle joined in unity are generated by the spectra of  $xP_{(123)} + (1-x)\mathbb{I}_3$ , see figure 2(b). The third vertical edge is obtained from the spectra of another interpolating family  $xP_{(123)} + (1-x)P_{(132)}$ , see figure 2(a). The boundary of  $\Sigma_3^B$  is obtained from spectra of the members of the convex polyhedron of the bistochastic matrices of size 3. On the other hand, the permutations  $P_{(123)}$  and  $P_{(12)(3)}$  do not commute, and the spectra of their linear combination form a curve inside  $\Sigma_3^B$ , see figure 2(c). To show that there are no points in the set  $\Sigma_N^B$  outside  $E_3$ , note that  $Z_2 \cup Z_3 = E_3 \subseteq \Sigma_3^B \subseteq \Sigma_3^S = E_3$ .

Let us move to the case  $N = 4$ . Two pairs of sides of the square forming  $Z_4$  constructed of commuting permutation matrices are shown in figures 2(d) and (e), while figure 2(f) presents the spectra of a combination of non-commuting permutation matrices, which interpolate between 3 and 4 permutations. This illustrates the fact that  $E_4$  is contained in the set  $\Sigma_4^B$ , but we have not succeeded in proving that both sets are equal.

The analysis of the support of the spectra of stochastic and bistochastic matrices can thus be summarized by

$$\bigcup_{k=2}^N Z_k = E_N \subseteq \Sigma_N^B \subseteq \Sigma_N^S = \tilde{E}_N \subseteq \bar{E}_N \tag{2.7}$$

where  $\tilde{E}_N$  is to remove the set-theoretical sum  $E_N$  of the regular polygons  $Z_k$  ( $k = 2, \dots, N$ ) supplemented by the area bounded by Karpelevich’s interpolation curves [27–29], whereas  $\bar{E}_N$  is the closed convex hull of  $E_N$ .

### 3. Majorization and entropy of bistochastic matrices

#### 3.1. Majorization

Consider two vectors  $\vec{x}$  and  $\vec{y}$ , consisting of  $N$  non-negative components each. Let us assume that they are normalized in a sense that  $\sum_{i=1}^N x_i = \sum_{i=1}^N y_i = 1$ . The theory of *majorization* introduces a partial order in the set of such vectors [3]. We say that  $\vec{x}$  is *majorized* by  $\vec{y}$ , written  $\vec{x} \prec \vec{y}$ , if

$$\sum_{i=1}^k x_i \leq \sum_{i=1}^k y_i \tag{3.1}$$

for every  $k = 1, 2, \dots, N$ , where we ordered the components of each vector in the decreasing order,  $x_1 \geq \dots \geq x_N$  and  $y_1 \geq \dots \geq y_N$ . Vaguely speaking, the vector  $\vec{x}$  is more ‘mixed’ than the vector  $\vec{y}$ .

The following theorem by Hardy, Littlewood and Polya applies the bistochastic matrices to the theory of majorization [3].

**Theorem 1 (HLP).** *For any vectors  $\vec{x}$  and  $\vec{y}$ , with the sum of their components normalized to unity,  $\vec{x} \prec \vec{y}$  if and only if*

$$\vec{x} = B\vec{y} \dots \text{for some bistochastic matrix } B. \tag{3.2}$$

It was later shown by Horn [31] that in the above theorem the word ‘bistochastic’ can be replaced by ‘orthostochastic’. In general, the orthostochastic matrix  $B$  satisfying the relation  $\vec{x} = B\vec{y}$  is not unique.

The functions  $f$ , which preserve the majorization order

$$\vec{x} \prec \vec{y} \quad \text{implies} \quad f(\vec{x}) \leq f(\vec{y}) \tag{3.3}$$

are called *Schur convex* [3]. Examples of Schur convex functions include  $h_q(\vec{x}) = \sum_{i=1}^N x_i^q$  for any  $q \geq 1$ , and  $h(\vec{x}) = \sum_{i=1}^N x_i \ln x_i$ .

The degree of mixing of the vector  $\vec{x}$  can be characterized by its Shannon entropy  $H$  or the generalized Rényi entropies  $H_q$  ( $q \geq 1$ ):

$$H(\vec{x}) = - \sum_{i=1}^N x_i \ln x_i \quad H_q(\vec{x}) = \frac{1}{1-q} \ln \left( \sum_{i=1}^N x_i^q \right). \tag{3.4}$$

In the limiting case one obtains  $\lim_{q \rightarrow 1} H_q(\vec{x}) = H(\vec{x})$ . If  $\vec{x}$  represents the non-negative eigenvalues of a density matrix,  $H$  is called the von Neumann entropy. Let  $\vec{x} = B\vec{y}$ . Due to the Schur-convexity we have  $H_q(\vec{x}) \geq H_q(\vec{y})$ , since we changed the sign and reversed the direction of inequality. An interesting application of the theory of majorization in the space



of density matrices representing mixed quantum states has recently been provided by Nielsen [14]. Consider a mixed state  $\rho$  with the spectrum consisting of non-negative eigenvalues  $\lambda_1 \geq \dots \geq \lambda_N$ , which sum to unity. This state may be written as a mixture of  $N$  pure states,  $\rho = \sum_{i=1}^N p_i |\psi_i\rangle\langle\psi_i|$  if and only if  $\vec{p} \prec \vec{\lambda} = (\lambda_1, \dots, \lambda_N)$ , where  $\vec{p} = (p_1, \dots, p_k)$  (if both vectors have different length, the shorter is extended by a sufficient number of extra components equal to zero). This statement is not true if the pure states  $|\psi_i\rangle$  are required to be distinct [32].

Consider now the non-unitary dynamics of the density operators given by  $\rho \rightarrow \rho' = \sum_{j=1}^L q_j U_j \rho U_j^\dagger$ . This process, called *random external fields* [33], is described by  $L$  unitary operations  $U_j$  ( $j = 1, \dots, L$ ) and non-negative probabilities satisfying  $\sum_{j=1}^L q_j = 1$ . Denoting respective spectra, ordered decreasingly, by  $\vec{\lambda}$  and  $\vec{\lambda}'$  one can find unistochastic matrix  $B$  such that  $\vec{\lambda}' = B\vec{\lambda}$ , so due to the HLP theorem we have  $\vec{\lambda}' \prec \vec{\lambda}$  [15, 34]. Therefore, after each iteration the mixed state becomes more mixed and its von Neumann entropy is non-decreasing.

### 3.2. Preorder in the space of bistochastic matrices

A bistochastic matrix  $B$  acting on a probability vector  $\vec{x}$  makes it more mixed and increases its entropy. To settle which bistochastic matrices have stronger mixing properties, one may introduce a relation (preordering) in the space of bistochastic matrices [35] writing

$$B_1 \prec B_2 \quad \text{iff} \quad B_1 = BB_2 \text{ for some bistochastic matrix } B. \quad (3.5)$$

We have already distinguished some bistochastic matrices: permutation matrices  $P$  with only  $N$  non-zero elements, and the uniform van der Waerden matrix  $B_*$ , with all its  $N^2$  elements equal to  $1/N$ . For an arbitrary bistochastic matrix  $B$  and for all permutation matrices  $P$  we have  $B_* = B_*B$  and  $B = (BP^{-1})P$ , and hence  $B_* \prec B \prec P$ . The relation  $B_1 \prec B_2$  implies  $B_1\vec{y} \prec B_2\vec{y}$  for every probability vector  $\vec{y}$ , but the converse is not true in general (see [36, 37]).

### 3.3. Entropy of bistochastic matrices

To measure mixing properties of a bistochastic matrix  $B$  of size  $N$  one may consider its entropy. We define the *Shannon entropy* of  $B$  as the mean entropy of its columns (rows), which is equivalent to

$$H(B) := -\frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N B_{ij} \ln B_{ij}. \quad (3.6)$$

As usual, in the definitions of entropy we set  $0 \ln 0 = 0$ , if necessary. The entropy changes from zero for permutation matrices to  $\ln N$  for the uniform matrix  $B_*$ .

Due to the majorization of each column vector, the relation  $C \prec B$  implies  $H(B) \leq H(C)$ , but the converse is not true. To characterize quantitatively the effect of entropy increase under the action of a bistochastic matrix  $B$ , let us define the *weighted entropy* of matrix  $B$  with respect to a probability vector  $\vec{y} = (y_1, \dots, y_N)$ :

$$H_{\vec{y}}(B) := \sum_{k=1}^N y_k H(B_k) = -\sum_{k=1}^N y_k \sum_{j=1}^N B_{jk} \ln B_{jk} \quad (3.7)$$

where  $B_k$  is a probability vector defined by  $B_k := (B_{1k}, \dots, B_{Nk})$  for  $k = 1, \dots, N$ . In this notation  $H(B) = H_{e_*}(B)$ , where  $e_* = (1/N, \dots, 1/N)$ . The weighted entropy allows one to write down the following bounds for  $H(B\vec{y})$ :

$$\max\{H(\vec{y}), H_{\vec{y}}(B)\} \leq H(B\vec{y}) \leq H(\vec{y}) + H_{\vec{y}}(B) \tag{3.8}$$

the proof of which is provided elsewhere [38]. These bounds have certain implications in quantum mechanics. For example, if a non-unitary evolution of the density operator under the action of random external field is considered [14], they tell us how much the von Neumann entropy of the mixed state may grow during each iteration.

Using the above proposition we shall show that the entropy of bistochastic matrices is subadditive. Namely, the following theorem holds.

**Theorem 2.** *Let  $B$  and  $C$  be two bistochastic matrices. Then*

$$\max\{H(B), H(C)\} \leq H(BC) \leq H(B) + H(C) \tag{3.9}$$

and, analogously,

$$\max\{H(B), H(C)\} \leq H(CB) \leq H(B) + H(C). \tag{3.10}$$

**Proof.** Consider stochastic vectors  $\vec{y}_n := (C_{1n}, \dots, C_{Nn})$  for  $n = 1, \dots, N$  (the rows of the matrix  $C$ ). Applying (3.8) we get

$$\max(H_{\vec{y}_n}(B), H(\vec{y}_n)) \leq H(B\vec{y}_n) \leq H_{\vec{y}_n}(B) + H(\vec{y}_n).$$

Hence

$$\max\left(\sum_{k=1}^N C_{kn} \sum_{j=1}^N \eta(B_{jk}), \sum_{k=1}^N \eta(C_{kn})\right) \leq \sum_{k=1}^N \eta\left(\sum_{j=1}^N B_{kj} C_{jn}\right)$$

and

$$\sum_{k=1}^N \eta\left(\sum_{j=1}^N B_{kj} C_{jn}\right) \leq \sum_{k=1}^N C_{kn} \sum_{j=1}^N \eta(B_{jk}) + \sum_{k=1}^N \eta(C_{kn})$$

where  $\eta(x) = -x \ln x$  for  $x > 0$ . Multiplying the above inequalities by  $1/N$  and summing over  $n = 1, \dots, N$ , we get (3.9). We obtain (3.10) in an analogous way.  $\square$

#### 4. Ensembles of random unistochastic matrices

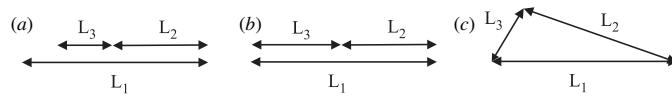
##### 4.1. Unistochastic matrices

To demonstrate that a given bistochastic matrix  $B$  is unistochastic one needs to find a unitary matrix  $U$  such that  $B_{ij} = |U_{ij}|^2$ . In other words one needs to find a solution of the coupled set of non-linear equations enforced by the unitarity  $UU^\dagger = U^\dagger U = \mathbb{I}$ ,

$$\sum_{j=1}^N \sqrt{B_{jk} B_{jl}} \exp(i(\phi_{jk} - \phi_{jl})) = \delta_{kl} \quad \text{for all } 1 \leq k \leq l \leq N \tag{4.1}$$

for the unknown phases of each complex element  $U_{jk} = \sqrt{B_{jk}} e^{i\phi_{jk}}$ . The diagonal constraints for  $k = l$  are fulfilled, since  $B$  is bistochastic.

For  $N = 2$  all bistochastic matrices are orthostochastic (see e.g. equation (4.6)), and so  $\Omega_2^B = \Omega_2^U = \Omega_2^O$ . This is not the case for higher dimensions, for which there exist



**Figure 3.** Chain rule for unistochasticity for  $N = 3$  (see (4.3) and (4.4)): (a) the longest link  $L_1 > L_2 + L_3$  so the matrix  $B$  is not unistochastic, (b) condition for orthostochasticity  $L_1 = L_2 + L_3$ , and (c) weaker condition for unistochasticity  $L_1 \leq L_2 + L_3$ .

bistochastic matrices which are not unistochastic, and so  $\Omega_N^U \subsetneq \Omega_N^B$  for  $N \geq 3$ . Thus  $\Omega_N^U$  is not a convex set for  $N \geq 3$ , since it contains all the permutation matrices and is smaller than their convex hull, which, according to the Birkhoff theorem, is equal to  $\Omega_N^B$ . Simple examples of bistochastic matrices which are not unistochastic were already provided (for  $N = 3$ ) by Schur and Hoffman (see e.g. [3]),

$$B_1 = \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix} \quad B_2 = \frac{1}{6} \begin{bmatrix} 0 & 3 & 3 \\ 3 & 1 & 2 \\ 3 & 2 & 1 \end{bmatrix}. \tag{4.2}$$

To see that there exists no corresponding unitary matrix  $U$ , we shall analyse constraints implied by the unitarity. Define vectors containing square roots of the column (row) entries, e.g.,  $\vec{v}_k := \{\sqrt{B_{k1}}, \sqrt{B_{k2}}, \dots, \sqrt{B_{kN}}\}$ . The scalar products of any pair of any two different vectors  $\vec{v}_k \cdot \vec{v}_l$  consist of  $N$  terms,  $L_n = \sqrt{B_{kn}B_{ln}}$ ,  $n = 1, \dots, N$  which for unistochastic  $B$  have to fulfill the triangle inequality according to (4.1). In the case of  $B_1$  from (4.2) the scalar product related to the two first columns ( $\vec{v}_1, \vec{v}_2$ ) consists of three terms  $L_1 = 1, L_2 = L_3 = 0$ , which do not satisfy the triangle inequality. Thus it is not possible to find the corresponding phases  $\phi_{jk}$  satisfying (4.1). This observation allows us to obtain a set of *necessary* conditions a bistochastic  $B$  must satisfy to be unistochastic [11]:

$$\max_{m=1, \dots, N} \sqrt{B_{mk}B_{ml}} \leq \frac{1}{2} \sum_{j=1}^N \sqrt{B_{jk}B_{jl}} \quad \text{for all } 1 \leq k < l \leq N \tag{4.3}$$

and

$$\max_{m=1, \dots, N} \sqrt{B_{km}B_{lm}} \leq \frac{1}{2} \sum_{j=1}^N \sqrt{B_{kj}B_{lj}} \quad \text{for all } 1 \leq k < l \leq N. \tag{4.4}$$

We shall refer to the above inequalities as the ‘chain rule’: the longest link  $L_1$  of a closed chain cannot be longer than the sum of all other links  $L_2 + \dots + L_N$ , see figure 3. The set of  $N(N - 1)/2$  conditions (4.3) (respectively (4.4)) treats all possible pairs of the columns (respectively rows) of  $B$ . Only for  $N = 3$  both sets of conditions are equivalent (since equations (4.1) for the phases may be separated [39]), but for  $N \geq 4$  there exist matrices which satisfy only one class of the constraints. For example, a bistochastic matrix

$$B_4 = \frac{1}{100} \begin{bmatrix} 1 & 17 & 25 & 57 \\ 38 & 38 & 24 & 0 \\ 42 & 5 & 29 & 24 \\ 19 & 40 & 22 & 19 \end{bmatrix} \tag{4.5}$$

found by Pakoński [39] satisfies the row conditions (4.4), but violates the column conditions (4.3), so cannot be unistochastic (the third term of the product of the roots of the first and the fourth columns is larger than the sum of the remaining three terms). It is easy to see that for an arbitrary  $N$  these necessary conditions are satisfied by any bistochastic  $B$  sufficiently close

to the van der Waerden matrix  $B_*$ , for which all links of the chain are equal,  $L_i = 1/N$ . It is then tempting to expect that there exists an open vicinity of  $B_*$  included in  $\Omega_N^U$ , i.e.  $B_*$  lies in the interior of  $\Omega_N^U$  and, consequently,  $\Omega_N^U$  has positive volume. Certain conditions *sufficient* for unistochasticity were already found by Au-Yeung and Cheng [40], but they do not answer the question concerning the volume of  $\Omega_N^U$ . On the other hand, it is well known that the set of unistochastic matrices is connected and compact [41], and is not dense in the set of bistochastic matrices [42].

To analyse the properties of bistochastic matrices, it is convenient to introduce so called  $T$ -transforms, which in a sense reduce the problem to two dimensions. A  $T$ -transform acts as the identity in all but two dimensions, in which it has a common form of an orthostochastic matrix

$$\tilde{T}(\varphi) = \begin{bmatrix} \cos^2 \varphi & \sin^2 \varphi \\ \sin^2 \varphi & \cos^2 \varphi \end{bmatrix} \quad \text{such that} \quad \tilde{O}_2(\varphi) = \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix} \quad (4.6)$$

is orthogonal and  $\tilde{T}(\varphi)_{ij} = \tilde{O}_2(\varphi)_{ij}^2$  for  $i, j = 1, 2$ . Any matrix  $B$  obtained as a sequence of at most  $(N - 1)$   $T$ -transforms,  $B = T_{N-1} \cdots T_2 T_1$ , where each  $T_k$  acts in the two-dimensional subspace spanned by the base vectors  $k$  and  $k + 1$ , is orthostochastic. To show this it is enough to observe that each element of  $B$  is a product of non-trivial elements of the transformations  $T_k$ . Hence taking its square root and adjusting the signs, one may find a corresponding orthogonal matrix defined by the products of the elements of  $\tilde{O}_k$  [3, 6, 16]. Although any product of an arbitrary number of  $T$ -transforms satisfies the chain-links conditions [32], for  $N \geq 4$  there exist products of a finite number of  $T$ -transforms (also called *pinching matrices*) which are not unistochastic [43]. In the same paper it is also shown that there exist unistochastic matrices which cannot be written as a product of  $T$ -transforms.

Consider a unistochastic matrix  $B$  and the set  $\mathcal{U}_B \subset U(N)$  of all unitary matrices corresponding to  $B$  in the sense that  $B_{ij} = |U_{ij}|^2$  for  $i, j = 1, \dots, N$ . Such sets endowed with appropriate probability measures play a role in the theory of quantum graphs [10–12] and were called *unitary stochastic ensembles* by Tanner [12]. It is easy to see that these sets are invariant under the operations  $U \rightarrow V_1 U V_2$ , where  $V_1$  and  $V_2$  are arbitrary diagonal unitary matrices. The dimensionality arguments suggest that, having  $U \in \mathcal{U}_B$  fixed, each element of  $\mathcal{U}_B$  can be obtained in this way [44]. However, in general this conjecture is false and for certain bistochastic matrices  $B$  the set  $\mathcal{U}_B$  is larger. This is shown in appendix A, in which a counterexample for  $N = 4$  is provided.

#### 4.2. Definition of ensembles

To analyse random unistochastic matrices, one needs to specify a probability measure in this set. As already discussed in the introduction, unistochastic ensemble (USE) and orthostochastic ensemble (OSE) can be defined with the help of the Haar measure on the group of unitary matrices  $U(N)$  and orthogonal matrices  $O(N)$ , respectively [19]. In other words the bistochastic matrices

$$B_{ij}^U := |U_{ij}|^2 \quad \text{and} \quad B_{ij}^O := (O_{ij})^2 \quad (4.7)$$

pertain to USE and OSE respectively, if the matrices  $U$  and  $O$  are generated with respect to the Haar measures on the unitary (orthogonal) group.

Dynamical systems with time reversal symmetry are described by unitary symmetric matrices [45]. The ensemble of these matrices, defined by  $W = U U^T$ , is invariant with respect to orthogonal rotations and is called the *circular orthogonal ensemble* (COE). In an

analogous way we may thus define the following three ensembles of symmetric bistochastic matrices (SBM):

$$\begin{aligned}
 \text{(a) } S_1 &:= BB^T & \text{so } S_{ij} &:= \sum_{k=1}^N |U_{ik}|^2 |U_{jk}|^2, \\
 \text{(b) } S_2 &:= \frac{1}{2}(B + B^T) & \text{so } S_{ij} &= \frac{1}{2}(|U_{ij}|^2 + |U_{ji}|^2), \\
 \text{(c) } S_3 &:= |W_{ij}|^2 = |(UU^T)_{ij}|^2 & \text{so } S_{ij} &:= \left| \sum_{k=1}^N U_{ik} U_{jk} \right|^2,
 \end{aligned} \tag{4.8}$$

where bistochastic matrices  $B$  are generated according to USE (or, equivalently, unitary matrices  $U$  are generated according to CUE).

### 4.3. Spectra of random unistochastic matrices

Since the sets of the bi-, uni-, and (ortho-)stochastic matrices are related by the inclusion relations:  $\Omega_N^O \subseteq \Omega_N^U \subseteq \Omega_N^B \subseteq \Omega_N^S$ , analogous relations must hold for the supports of their spectra,  $\Sigma_N^O \subseteq \Sigma_N^U \subseteq \Sigma_N^B \subseteq \Sigma_N^S$ . For  $N = 2$  the spectrum of a bistochastic matrix must be real. The subleading eigenvalue  $\lambda_2 = 2B_{11} - 1$ , which allows one to obtain the distributions along the real axis. For USE the respective density is constant,  $P_r(\lambda) = 1/4$  while for OSE it is given by the formula  $P_r(\lambda) = 1/(2\pi\sqrt{1-\lambda^2})$  for  $\lambda \in (-1, 1)$ . These densities are normalized to  $1/2$ , since for any random matrix its leading eigenvalue is equal to unity.

For larger matrices we generated random unitary (orthogonal) matrices with respect to the Haar measure by means of the Hurwitz parametrization [46] as described in [47, 48]. Squaring each element of the matrices generated in this way, we get random matrices typical for USE (OSE). In general, the density of the spectrum of random uni-, (ortho-)stochastic matrices may be split into three components:

- (a) two-dimensional density with the domain forming a subset  $\Sigma_N^U$  ( $\Sigma_N^O$ ) of the unit circle;
- (b) one-dimensional density at the real line described by the function  $P_r(x)$  for  $x \in [-1, 1]$ ;
- (c) the Dirac delta  $\frac{1}{N}\delta(z - 1)$  describing the leading eigenvalue, which exists for every unistochastic matrix.

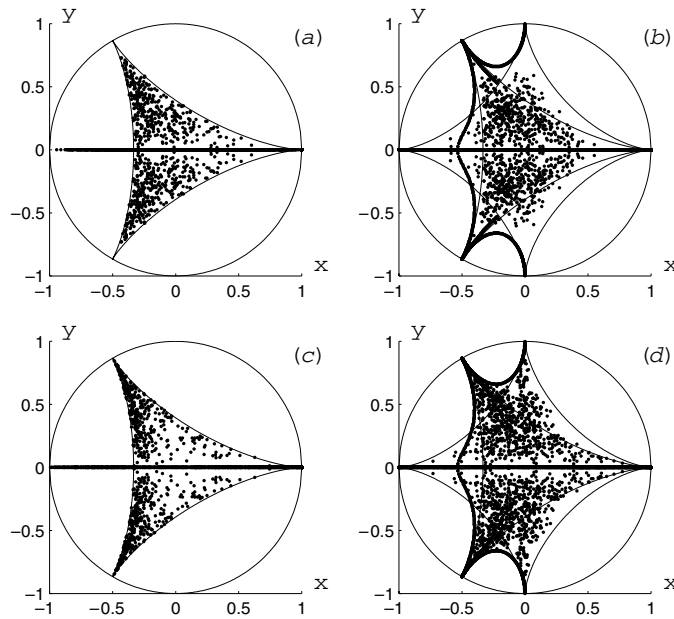
Based on the numerical results presented in figure 4(a), we conjecture that  $\Sigma_3^U = \Sigma_3^O$  and consists of a real interval (already present for  $N = 2$ ) and the inner part of the 3-hypocycloid. This curve is drawn by a point at a circle of radius  $1/3$ , which rolls (without sliding) inside the circle of radius 1. The parametric formula reads

$$\begin{cases} x = \frac{1}{3}(2 \cos \phi + \cos 2\phi) \\ y = \frac{1}{3}(2 \sin \phi - \sin 2\phi) \end{cases} \tag{4.9}$$

where  $\phi \in [0, 2\pi)$ .

To find the unistochastic matrices with spectra at the cycloid, consider a two-parameter family of combinations of permutation matrices  $a^2\mathbb{I} + b^2P + c^2P^2$  with  $a^2 + b^2 + c^2 = 1$ . Here  $P$  represents the non-trivial three elements permutation matrix,  $P = P_{(123)}$ , so  $P^3 = \mathbb{I}$ . The one-parameter family of these bistochastic matrices, which satisfy the condition for unistochasticity, produces spectra located along the entire hypocycloid. Consider the matrices

$$O_3(\varphi) := \begin{bmatrix} a & b & c \\ c & a & b \\ b & c & a \end{bmatrix} \quad \text{and} \quad B_3(\varphi) := \begin{bmatrix} a^2 & b^2 & c^2 \\ c^2 & a^2 & b^2 \\ b^2 & c^2 & a^2 \end{bmatrix} \tag{4.10}$$



**Figure 4.** Spectra of random unistochastic matrices of size (a)  $N = 3$  (1200 matrices) and (b)  $N = 4$  (800 matrices), spectra of random orthostochastic matrices of size (c)  $N = 3$  (1200 matrices) and (d)  $N = 4$  (800 matrices). Thin lines denote 3- and 4-hypocycloids, while the thick lines represent the 3-4 interpolation arc (part of it is shown in figure 2(f)).

where their elements depend on a single parameter  $\varphi \in [0, 2\pi)$  and

$$\begin{cases} a = a(\varphi) = -\frac{1}{3}(1 + 2 \cos \varphi) \\ b = b(\varphi) = \frac{1}{3}(\cos \varphi - 1) + \frac{1}{\sqrt{3}} \sin \varphi \\ c = c(\varphi) = \frac{1}{3}(\cos \varphi - 1) - \frac{1}{\sqrt{3}} \sin \varphi. \end{cases} \quad (4.11)$$

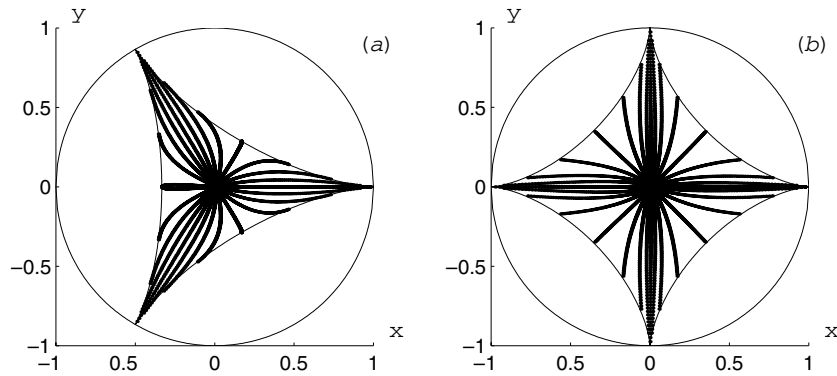
It is easy to see that  $a^2 + b^2 + c^2 = 1$  and  $ab + bc + ca = 0$ , so  $O_3$  is orthogonal and  $B_3$  is orthostochastic. Simple algebra shows that the spectrum of  $B_3(\varphi)$  forms the 3-hypocycloid given by (4.9), see appendix B.

An alternative approach, based on exponentiation of permutation matrices, leads to unistochastic matrices with spectrum on a hypocycloid. Let  $P_N := P_{(12\dots N)}$  be the non-trivial permutation matrix of size  $N$ . Since  $P_N$  is unitary, so is its power  $(P_N)^\alpha$ . We define it for an arbitrary real exponent by  $(P_N)^\alpha := U^\dagger D^\alpha U$ , where  $U$  is a unitary matrix diagonalizing  $P_N$  and  $D$  represents the diagonal matrix of its eigenvalues—it is assumed that the eigenphases of such a matrix belong to  $[0, 2\pi)$ . Since  $P_N^0 = \mathbb{1}_N$ , one may expect that defining the corresponding bistochastic matrices and varying the exponent  $\alpha$  from zero to unity, one obtains an arc of a hypocycloid. This fact is true as shown in appendix C, in which we prove a general result, valid for an arbitrary matrix size.

**Proposition 3.** *The spectra of the family of unistochastic matrices of size  $N$*

$$B_{ij}^{(N,\alpha)} := \left| (P_N^\alpha)_{ij} \right|^2 \quad \text{with } \alpha \in [0, N/2] \quad (4.12)$$

*generate the  $N$ -hypocycloid (and inner diagonal hypocycloids of the radius ratio  $k/N$  with  $k = 2, \dots, N - 1$ ).*



**Figure 5.** Spectra of a family of bistochastic matrices obtained by squaring elements of unitary matrices  $(P_N^\alpha)^\beta (F^{(N)})^{1-\beta}$  with  $\beta \in [0, 1]$  and (a)  $N = 3$ , the curves are labelled by  $\alpha = 0, 1/8, 2/8, \dots, 3/2$  and (b)  $N = 4, \alpha = 0, 1/8, 2/8, \dots, 2$ . For reference we have plotted the hypocycloids with a thin line.

Let  $H_N$  denote the set bounded by the  $N$ -hypocycloid. Figure 4(c) suggests that  $H_3$  is contained in  $\Sigma_3^O$ . This conjecture may be supported by considering the spectra interpolating between the origin  $(0, 0)$  and a selected point on the hypocycloid. To find such a family we shall use the Fourier matrix  $F^{(N)}$  of size  $N$  with elements  $F_{kl}^{(N)} := \exp(-2kl\pi i/N)/\sqrt{N}$ . Since amplitudes of all elements of this matrix are equal, the corresponding bistochastic matrix equals the van der Waerden matrix  $B_*$  for which all subleading eigenvalues vanish. The matrix  $P_N^\alpha$  generates a unistochastic matrix  $B^{(N,\alpha)}$  with an eigenvalue at the hypocycloid, so the family of unistochastic matrices related to  $(P_N^\alpha)^\beta (F^{(N)})^{1-\beta}$  provides an interpolation between the origin and a selected point on the hypocycloid, see figure 5. In other words, we conjecture that the spectra of a two-parameter family of unistochastic matrices obtained from  $(P_N^\alpha)^\beta (F^{(N)})^{1-\beta}$  explore the entire  $H_N$ .

Numerical results obtained for  $N = 3$  random uni-, (ortho-)stochastic matrices allow us to claim that there are no complex eigenvalues outside the 3-hypocycloid, so that  $\Sigma_3^U = \Sigma_3^O = H_2 \cup H_3$ . Interestingly,  $H_3$ , the 3-hypocycloid and its interior, determines the set of all unistochastic matrices which belong to the cross section of  $\Omega_3^B$  defined by the plane spanned by  $P_3, P_3^2$  and  $P_3^3 = \mathbb{I}$  [32], see also appendix B.

Numerical results for spectra of random uni- (ortho-)stochastic matrices for  $N = 4$  are shown in figures 4(b) and (d). The set  $\Sigma_4^U$  includes the entire set  $\Sigma_3^U$ , but also the 4-hypocycloid, sometimes called *asteroid*, and formed by the solutions of the equation

$$x^{2/3} + y^{2/3} = 1. \tag{4.13}$$

More generally, the spectra of orthostochastic matrices of size  $N$  contain the  $N$ -hypocycloid  $H_N$

$$\begin{cases} x = \frac{1}{N}[(N-1)\cos\phi + \cos(N-1)\phi] \\ y = \frac{1}{N}[(N-1)\sin\phi - \sin(N-1)\phi] \end{cases} \tag{4.14}$$

with a corner at 1, as proved in appendix B. The set  $\Sigma_N^U$  consists of the sets bounded by hypocycloids of a smaller dimension, which we denote by  $G_N := \bigcup_{k=2}^N H_k$ .

However, as seen in figure 4(b) for  $N = 4$  there exist some eigenvalues of unistochastic or even orthostochastic matrices outside this set. In fact one needs to find interpolations between roots of unity of different orders (the corners of  $k$ - and  $n$ -hypocycloids) based on the families

of orthostochastic matrices. Such a family interpolating between the corners of  $H_3$  and  $H_4$  is plotted in figure 2(f), since these bistochastic matrices are orthostochastic. A general scheme for finding the required interpolations is based on the fact that if  $O(\varphi)$  is a family of orthogonal matrices and  $B_{ij}(\varphi) = O_{ij}^2(\varphi)$  is the corresponding family of orthostochastic matrices, then another such family is produced by the multiplication by some permutation matrix  $P$ :  $O'(\varphi) = O(\varphi)P$ . For example, if the matrix  $O_4(\varphi)$  of size 4 contains elements  $O_{11} = O_{22} = 1$  and the block diagonal matrix  $O_2(\varphi)$  (see (4.6)), then the squared elements of the orthogonal matrices  $O_4(\varphi)P_{(1234)}$  provide orthostochastic matrices, the spectra of which form the 3–4 interpolating curve contained in  $E_4$  and plotted in figures 2(f) and 4(d). To obtain orthostochastic matrices, the spectra of which provide the curve which joins both complex corners of  $H_3$  and is not contained in it (see figure 4(d)), one should take the orthogonal matrix  $O_{3,1}(\varphi)$  of size 4 with  $O_{11} = 1$  which contains the block diagonal matrix  $O_3(\varphi)$  (4.10), and create bistochastic matrices out of  $O_{3,1}(\varphi)P_{(12)(34)}$ . The exact form of such families of orthostochastic matrices is provided in appendix D.

Let  $\tilde{G}_N$  denote the set  $G_N$  extended by adding the regions bounded by the interpolations between all neighbouring corners of  $H_k$  and  $H_n$  with  $k < n \leq N$  constructed in an analogous way as for  $N = 4$ . The sequence of hypocycloids with neighbouring corners is given by the order of fractions present in the *Farey sequence* and *Farey tree* [49]. Our investigation of the support of the spectra of unistochastic and orthostochastic matrices may be concluded by a relation analogous to (2.7)

$$\bigcup_{k=2}^N H_k := G_N \subset \Sigma_N^O \simeq \Sigma_N^U \simeq \tilde{G}_N \subset E_N =: \bigcup_{k=2}^N Z_k \tag{4.15}$$

where the sign  $\simeq$  represents the conjectured equality. Numerical results suggest that the support  $\Sigma_N$  is the same for both ensembles: USE and OSE. However, the density of eigenvalues  $P(z)$  is different for uni- and (ortho-)stochastic ensembles. The repulsion of the complex eigenvalues from the real line is more pronounced for the orthostochastic ensemble, as demonstrated in figures 4(b) and (d).

The larger the  $N$ , the better the domains  $\Sigma_N^O$  and  $\Sigma_N^U$  fill the unit disk. On the other hand, the eigenvalues of a large modulus are unlikely; the density  $P(z)$  is concentrated in a close vicinity of the origin,  $z = 0$ . Moreover, in this case the weight of the singular part of the density at the real line decreases with the matrix size  $N$ . To characterize the spectrum qualitatively, we analysed the densities of the distributions  $P_k(r)$  of the moduli of the largest eigenvalues  $\lambda_k$ . The results obtained for random unistochastic matrices are shown in figure 6(a). Figure 6(b) shows analogous data for the singular values  $\sigma_i$  of  $B$ -per definition square roots of the real eigenvalues of the symmetric matrices  $BB^T$  [50]. Since the singular values bound moduli of eigenvalues from above [50], the distribution  $P(\sigma)$  is localized at larger values than  $P(r)$ . Thus the expectation values satisfy  $\langle r_k \rangle < \langle \sigma_k \rangle$  as shown in figures 6(c) and (d). The modulus of the second eigenvalue decreases with matrix size as  $N^{-1/2}$ . These results are consistent with the recent work of Berkolaiko [19], who suggested describing the distribution  $P_2(r)$  by the generalized extreme value distribution [51].

#### 4.4. Average entropy

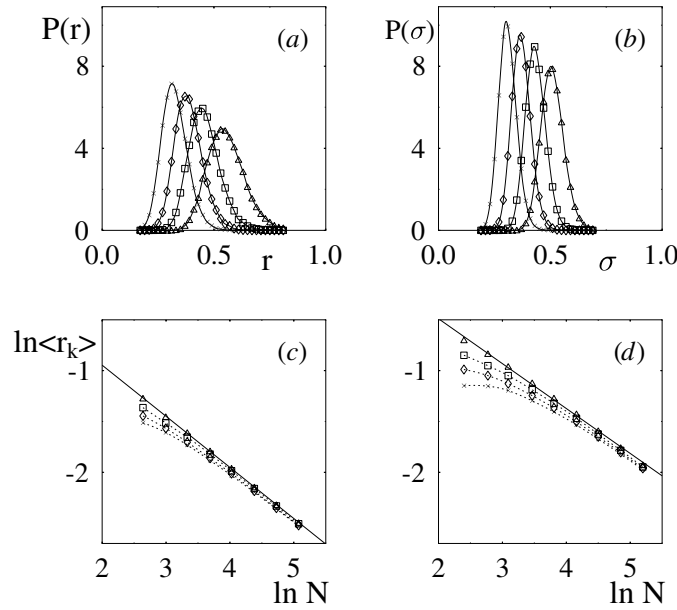
We can compute the mean entropy averaged over the ensembles of unistochastic or orthostochastic matrices. Clearly we have

$$\langle H \rangle_{\text{USE}} = N \langle -|U_{ij}|^2 \ln |U_{ij}|^2 \rangle_{\text{CUE}} \tag{4.16}$$

and

$$\langle H \rangle_{\text{OSE}} = N \langle -|O_{ij}|^2 \ln |O_{ij}|^2 \rangle_{\text{COE}} \tag{4.17}$$





**Figure 6.** Unistochastic ensemble. Distribution of the modulus of the second ( $\Delta$ ), third ( $\square$ ), fourth ( $\diamond$ ) and fifth ( $\times$ ) largest eigenvalues (a) and singular value (b) (lines are drawn to guide the eye). Expectation values for  $k = 2, 3, 4, 5$  of the subleading (c) eigenvalues and (d) singular values as a function of the matrix size  $N$ . Exponential fits, represented by solid lines, give  $\langle r_2 \rangle \approx N^{-0.503}$  and  $\langle \sigma_2 \rangle \approx N^{-0.446}$ .

where  $U_{ij}$  and  $O_{ij}$  are entries of unitary or orthogonal matrices, respectively. The exact formulae for the above averages were obtained by Jones in [52, 53]. Using these results we get

$$\langle H \rangle_{\text{USE}} = \Psi(N+1) - \Psi(2) = \sum_{k=2}^N \frac{1}{k} \quad (4.18)$$

and

$$\langle H \rangle_{\text{OSE}} = \Psi(N/2+1) - \Psi(3/2) = \begin{cases} 2 \ln 2 - 2 + \sum_{l=1}^k \frac{1}{l} & N = 2k \\ 2 \sum_{l=1}^k \frac{1}{2l+1} & N = 2k+1 \end{cases}, \quad (4.19)$$

where  $\Psi$  denotes the digamma function. For large  $N$  the digamma function behaves logarithmically,  $\Psi(N) \sim \ln N$ , and both averages display similar asymptotic behaviour  $\langle H \rangle_{\text{USE}} \approx \ln N - 1 + \gamma$  and  $\langle H \rangle_{\text{OSE}} \approx \ln N - 2 + \gamma + \ln 2$ , where  $\gamma \approx 0.577$  stands for the Euler constant. Note that both averages are close to the maximal value  $\ln N$ , attained for orthostochastic matrices corresponding to  $B_*$ , and their difference  $\langle H \rangle_{\text{USE}} - \langle H \rangle_{\text{OSE}}$  converges to  $1 - \ln 2 \approx 0.307$ .

#### 4.5. Average traces

Traces of consecutive powers of bistochastic matrices,  $\text{tr} B^n$ , are quantities important in applications related to *quantum chaos* [9]. In the following we evaluate the traces  $t_{N,n} := \langle \text{tr} B^n \rangle_{\text{USE}}$ , averaged over the unistochastic ensemble.

The spectrum of a bistochastic matrix of size 2 is real and may be written as  $\text{Sp}(B) = \{1, y\}$  with  $y \in [-1, 1]$ . For the unistochastic ensemble  $y = \cos 2\theta$ , where the angle  $\theta$  is distributed uniformly,  $P(\theta) = 2/\pi$  for  $\theta \in [0, \pi/2]$ . The average traces may be readily expressed by the moments  $\langle y^k \rangle$  for  $k \in \mathbb{N}$ , namely,

$$t_{2,2k+1} = 1 + \langle y^{2k+1} \rangle = 1 \quad t_{2,2k} = 1 + \langle y^{2k} \rangle = \frac{2k + 2}{2k + 1}. \tag{4.20}$$

Since the average size of all the diagonal elements must be equal,  $\langle |U_{ii}|^2 \rangle = 1/N$ , so the average trace  $t_{N,1} = \langle \sum_{i=1}^N |U_{ii}|^2 \rangle = 1$  and does not depend on the matrix size. Using the results of Mello [54], who computed several averages over the Haar measure on the unitary group  $U(N)$ , we derive in appendix E the following formulae:

$$t_{N,2} = 1 + \frac{1}{N + 1} \quad \text{and} \quad t_{N,3} = \begin{cases} 1 & \text{for } N = 2 \\ 1 + \frac{2}{N^2 + 3N + 2} & \text{for } N \geq 3. \end{cases} \tag{4.21}$$

Analogous expressions for larger  $N$  may be explicitly written as functions of the Mello averages, but it is not simple to put them into a transparent form. Numerical results support a conjecture that for arbitrary  $N$  the average traces tend fast to unity and the difference  $t_{N,n} - 1$  behaves as  $N^{1-n}$ . This fact is related to the properties of the spectra discussed above: for large  $N$  the spectrum is concentrated close to the centre of the unit circle, so the contribution of all the subleading eigenvalues to the traces becomes negligible. Related results on average traces of the symmetric unistochastic matrices  $BB^T$  are provided in [19].

### 5. Closing remarks

In this paper we defined the entropy for bistochastic matrices and proved its subadditivity. We also analysed special classes of bistochastic matrices: the unistochastic and orthostochastic matrices, and introduced probability measures on these sets. We found a characterization of complex spectra of unistochastic matrices in the unit circle and discussed the size of their subleading eigenvalue, which determines the speed of the decay of correlation in the dynamical system described by the matrices under consideration. Unistochastic matrices find diverse applications in different branches of physics and it is legitimate to ask, how a physical system behaves, if it is described by a random unistochastic matrix [19]. Since we succeeded in computing mean values of some quantities (traces, entropy) averaged over the ensemble of unistochastic matrices, our results provide some information concerning this issue.

On the other hand, several problems concerning bi-, uni- and (ortho-)stochastic matrices remain open and we conclude this paper listing some of them.

- (a) Prove the conjecture that the union of the spectra of bistochastic matrices  $\Sigma_N^B$  is equal to the sum of regular polygons  $E_N$ , i.e.,  $\Sigma_N^B = E_N$ .
- (b) Prove that the support  $\Sigma_3^U$  of spectra of unistochastic matrices of size  $N = 3$  contains exactly the interval  $[-1, 1]$  and the set bounded by the 3-hypocycloid  $H_3$ , i.e.,  $\Sigma_3^U = G_3$ .
- (c) Find an analytical formula for the boundaries of the set  $\tilde{G}_N$  obtained from interpolations between the neighbouring corners of  $k$ -hypocycloids with  $k \leq N$ .
- (d) Show that the support  $\Sigma_N^U$  of the spectra of unistochastic matrices contains  $\tilde{G}_N$  and check whether both sets are equal, i.e.,  $\Sigma_N^U = \tilde{G}_N$ .
- (e) Show that the supports of spectra of uni- and (ortho-) stochastic matrices are the same, i.e.,  $\Sigma_N^U = \Sigma_N^O$ .
- (f) Calculate the probability distribution  $P_N(z)$  of complex eigenvalue ensembles for uni-(ortho-) stochastic matrices.

- (g) Compute the expectation value of the subleading eigenvalue  $\langle r_2 \rangle$ , averaged over the uni-(ortho-) stochastic ensemble.
- (h) Calculate averages over the unistochastic ensemble of other quantities characterizing ergodicity of stochastic matrices, including ergodicity coefficients analysed by Seneta [55] and entropy contraction coefficient introduced by Cohen *et al* [56].
- (i) Find necessary and sufficient conditions for a bistochastic matrix to be unistochastic.
- (j) Provide a full characterization of the set of all unitary matrices  $U$ , which lead to the same unistochastic matrix  $B$ , i.e.,  $B_{ij} = |U_{ij}|^2$  for  $i, j = 1, \dots, k$ .

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### Appendix A. Unistochastic matrices stemming from a given bistochastic matrix

Let us consider two unitary  $N \times N$  matrices  $U$  and  $W$  such that for all  $i, j = 1, \dots, N$ ,

$$|U_{ij}|^2 = |W_{ij}|^2 \quad (\text{A1})$$

i.e., the corresponding unistochastic matrices are the same. It is obvious that this happens if  $W = V_1 U V_2$  with  $V_1$  and  $V_2$  being unitary diagonal. However, the converse statement, i.e., (A1) implies the existence of two diagonal unitary matrices  $V_1$  and  $V_2$  such that  $U = V_1 W V_2$ , is false [44]. The plausibility of such a conjecture is based on the following dimensional argument: we have  $N^2$  real numbers  $u_{ij} := |U_{ij}|$  fulfilling  $2N - 1$  relations stemming from the normalization of the rows

$$\sum_{j=1}^N u_{ij}^2 = 1 \quad i = 1, \dots, N \quad (\text{A2})$$

and the columns

$$\sum_{i=1}^N u_{ij}^2 = 1 \quad j = 1, \dots, N \quad (\text{A3})$$

of the unitary matrix  $U$ . The number of independent relations is one less than the total number of equations in (A2) and (A3) since summing all equations in (A2) over  $i$  gives the same result as summing all equations in (A3) over  $j$ , namely  $N = \text{Tr}(U^\dagger U)$ . On the other hand, the left and right multiplications by unitary diagonal  $V_1$  and  $V_2$  introduce exactly  $2N - 1$  parameters (here the number of independent parameters is diminished by one from the number of non-zero elements of both  $D_1$  and  $D_2$  since in the resulting matrix only the differences of eigenphases of  $D_1$  and  $D_2$  appear, so we can always put one of the eigenphases of  $D_1$ , say, to zero without changing the result of the transformation  $W \mapsto V_1 W V_2$ ). The simplest counterexample we know involves the following unitary matrices  $U$  and  $W$ :

$$U = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -e^{i\alpha} & e^{i\alpha} \\ 1 & -1 & e^{i\alpha} & -e^{i\alpha} \\ 1 & 1 & -1 & -1 \end{bmatrix} \quad W = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & -e^{i\beta} & e^{i\beta} & -1 \\ 1 & e^{i\beta} & -e^{i\beta} & -1 \end{bmatrix} \quad (\text{A4})$$

with  $|U_{ij}|^2 = |W_{ij}|^2 = 1/4$ . It is a matter of simple explicit calculations to show that there are no unitary diagonal  $V_1$  and  $V_2$  fulfilling  $W = V_1 U V_2$ , if  $\alpha, \beta \in [0, 2\pi]$  and  $\alpha\beta \neq 0$ .

**Appendix B. Orthostochastic matrices with spectrum at hypocycloids**

In this appendix we construct orthostochastic matrices with spectra on  $N$ -hypocycloids. Consider the following  $N \times N$  permutation matrix

$$P := \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \end{bmatrix} \tag{B1}$$

where for simplicity the dimensionality index  $N$  has been omitted. We have  $P^N = \mathbb{I}$ ,  $P^n \neq \mathbb{I}$  for  $n < N$  and the eigenvalues of  $P$  equal  $\exp\left(\frac{2\pi i}{N}k\right)$ ,  $k = 0, 1, \dots, N - 1$ .

We shall discuss separately the cases of odd and even  $N$ .

First let  $N = 2K + 1$  and

$$O := \sum_{j=0}^{N-1} a_j P^j \quad B := \sum_{j=0}^{N-1} a_j^2 P^j. \tag{B2}$$

Observe that since  $P^m$  and  $P^n$  do not have common non-zero entries for  $m \neq n$ ,  $0 \leq m, n \leq N - 1$ , the elements of  $B$  are squares of the corresponding elements of  $O$ . The eigenvalues of  $O$  and  $B$  read, respectively,

$$\Lambda_k = \sum_{j=0}^{N-1} a_j \exp\left(\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N - 1 \tag{B3}$$

$$\lambda_k = \sum_{j=0}^{N-1} a_j^2 \exp\left(\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N - 1. \tag{B4}$$

Inverting the discrete Fourier transforms in (B3), we obtain

$$a_j = \frac{1}{N} \sum_{k=0}^{N-1} \Lambda_k \exp\left(-\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N - 1 \tag{B5}$$

which, upon substituting to (B4), gives the eigenvalues of  $B$  in terms of the eigenvalues of  $O$ ,

$$\begin{aligned} \lambda_k &= \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{l=0}^{N-1} \sum_{r=0}^{N-1} \Lambda_l \Lambda_r \exp\left(-\frac{2\pi i}{N}(l+r-k)j\right) \\ &= \frac{1}{N} \sum_{l=0}^{N-1} \sum_{r=0}^{N-1} \Lambda_l \Lambda_r \delta_{r,k-l} = \frac{1}{N} \sum_{l=0}^{N-1} \Lambda_l \Lambda_{k-l} \end{aligned} \tag{B6}$$

where the indices are counted modulo  $N$ .

Our aim is now to find a family of orthogonal matrices  $O(\phi)$  such that when  $\phi$  changes (from 0 to  $2\pi$ , say) the eigenvalue  $\lambda_0(\phi)$  renders the  $N$ -hypocycloid  $H_N$  in the complex plane, i.e.

$$\lambda_0(\phi) = \frac{1}{N} [(N - 1) e^{i\phi} + e^{-i(N-1)\phi}]. \tag{B7}$$

First observe that the desired result is achieved if

$$\Lambda_k = \exp[i(k - K)\phi] \quad k = 0, 1, \dots, 2K = N - 1. \quad (\text{B8})$$

Indeed

$$\begin{aligned} \lambda_0 &= \frac{1}{N} \sum_{l=0}^{N-1} \Lambda_l \Lambda_{-l} = \frac{1}{N} \left( \Lambda_0^2 + \sum_{l=1}^{N-1} \Lambda_l \Lambda_{-l} \right) = \frac{1}{N} \left( \Lambda_0^2 + \sum_{l=1}^{N-1} \Lambda_l \Lambda_{N-l} \right) \\ &= \frac{1}{N} \left( e^{-2iK\phi} + \sum_{l=1}^{N-1} e^{i(l-K)\phi} e^{i(N-l-K)\phi} \right) = \frac{1}{N} (e^{-i(N-1)\phi} + (N-1) e^{i(N-2K)\phi}) \end{aligned} \quad (\text{B9})$$

$$= \frac{1}{N} [(N-1) e^{i\phi} + e^{-i(N-1)\phi}]. \quad (\text{B10})$$

In order to construct an orthogonal matrix  $O$  with the spectrum (B8), it is enough to find an antisymmetric  $A$  with the eigenvalues

$$\mu_k = i(k - K) \quad k = 0, 1, \dots, 2K. \quad (\text{B11})$$

If  $A$  is a polynomial in  $P$  then so is  $O = \exp(A\phi)$ ; moreover,  $O$  is orthogonal and has the desired spectrum (B8). Let us thus write

$$A := \sum_{j=1}^K \alpha_j (P^j - P^{N-j}) \quad (\text{B12})$$

which is clearly antisymmetric, with the eigenvalues

$$\begin{aligned} \mu_k &= \sum_{j=1}^K \alpha_j \left[ \exp\left(\frac{2\pi i}{N}jk\right) - \exp\left(\frac{2\pi i}{N}(N-j)k\right) \right] = 2i \sum_{j=1}^K \alpha_j \sin\left(\frac{2\pi}{2K+1}kj\right) \\ &k = 0, 1, \dots, 2K. \end{aligned} \quad (\text{B13})$$

Obviously  $\mu_K = 0$  and  $\mu_{2k-k} = -\mu_k$ ,  $k = 0, 1, 2, \dots, K$ . To fulfil (B11) it is thus enough that

$$2 \sum_{j=1}^K \alpha_j \sin\left(\frac{2\pi}{2K+1}kj\right) = k - K \quad k = 1, 2, \dots, K. \quad (\text{B14})$$

Using

$$\sum_{j=1}^K \sin\left(\frac{2\pi}{2K+1}kj\right) \sin\left(\frac{2\pi}{2K+1}mj\right) = \frac{2K+1}{4} \delta_{mk} \quad (\text{B15})$$

we solve (B14) for  $\alpha_j$ ,

$$\alpha_j = \frac{2}{2K+1} \sum_{k=1}^K k - K \sin\left(\frac{2\pi}{2K+1}kj\right). \quad (\text{B16})$$

For  $N$  even,  $N = 2K$ , the construction is very similar. We introduce  $E := \text{diag}(1, 1, \dots, 1, -1)$  and define  $\tilde{P} := EP$  which has eigenvalues  $\exp\left(\frac{2\pi i}{N}\left(k + \frac{1}{2}\right)\right)$ ,  $k = 0, 1, \dots, N-1$ , and construct the matrix  $O$  as a polynomial in  $\tilde{P}$  rather than in  $P$ ,

$$\tilde{O} := \sum_{j=0}^{N-1} a_j \tilde{P}^j \quad (\text{B17})$$

with the eigenvalues

$$\tilde{\Lambda}_k = \sum_{j=0}^{N-1} a_j \exp\left(\frac{2\pi i}{N} \left(k + \frac{1}{2}\right) j\right) \quad k = 0, 1, \dots, N - 1. \quad (\text{B18})$$

The matrix  $B$  of the squared elements of  $O$  is, as previously, the following polynomial in  $P$ :

$$B := \sum_{j=0}^{N-1} a_j^2 P^j. \quad (\text{B19})$$

Using exactly the same method as above, we express the eigenvalues  $\lambda_k$  of  $B$  given in terms of  $\tilde{\Lambda}_j$ ,

$$\lambda_k = \frac{1}{N} \sum_{l=0}^{N-1} \tilde{\Lambda}_l \tilde{\Lambda}_{k-l+1}. \quad (\text{B20})$$

Now if

$$\tilde{\Lambda}_k = \exp\left[i \left(k - K + \frac{1}{2}\right) \phi\right] \quad k = 0, 1, \dots, 2K - 1 = N - 1 \quad (\text{B21})$$

then

$$\begin{aligned} \lambda_{N-1} &= \frac{1}{N} \sum_{l=0}^{N-1} \tilde{\Lambda}_l \tilde{\Lambda}_{N-l} = \frac{1}{N} \left( \tilde{\Lambda}_0^2 + \sum_{l=1}^{N-1} \tilde{\Lambda}_l \tilde{\Lambda}_{N-l} \right) \\ &= \frac{1}{N} \left( e^{-i(2K-1)\phi} + \sum_{l=1}^{N-1} e^{i(l-K+1/2)\phi} e^{i(N-l-K+1/2)\phi} \right) \\ &= \frac{1}{N} (e^{-i(N-1)\phi} + (N-1) e^{i(N-2K+1)\phi}) = \frac{1}{N} [(N-1) e^{i\phi} + e^{-i(N-1)\phi}]. \end{aligned} \quad (\text{B22})$$

In full analogy with the case of odd  $N$ , we look for an antisymmetric matrix  $\tilde{A}$  with the eigenvalues

$$\tilde{\mu}_k = i \left(k - K + \frac{1}{2}\right) \quad (\text{B23})$$

in the form of a polynomial in  $\tilde{P}$

$$\tilde{A} := 2^{1/2} \tilde{\alpha}_K \tilde{P}^K + \sum_{j=1}^K \tilde{\alpha}_j (\tilde{P}^j + \tilde{P}^{N-j}). \quad (\text{B24})$$

Since it is easy to check,  $(\tilde{P}^j)^T = -\tilde{P}^{N-j}$  for  $j = 1, 2, \dots, K$ , the matrix  $A$  is indeed antisymmetric for arbitrary real  $\tilde{\alpha}_j$ ,  $j = 1, 2, \dots, K$ . The eigenvalues of  $A$  read

$$\tilde{\mu}_k = 2^{1/2} i (-1)^k \tilde{\alpha}_K + 2i \sum_{j=1}^{K-1} \tilde{\alpha}_j \sin\left[\frac{\pi}{K} \left(k + \frac{1}{2}\right) j\right] \quad k = 0, 1, \dots, 2K - 1. \quad (\text{B25})$$

Using arguments similar to those in the odd  $N$  case, we conclude that the choice

$$\tilde{\alpha}_j = \frac{1}{K} \sum_{k=0}^{K-1} \left(k - K + \frac{1}{2}\right) \sin\left[\frac{\pi}{K} \left(k + \frac{1}{2}\right) j\right] \quad j = 1, 2, \dots, K - 1 \quad (\text{B26})$$

$$\tilde{\alpha}_K = -\frac{\sqrt{2}}{4} \quad (\text{B27})$$

leads to the desired result (B23) and, consequently, the  $2K$ -hypocycloid (B22).

### Appendix C. Unistochastic matrices with spectra at hypocycloids

The above constructed matrices with spectra on  $N$ -hypocycloids were *orthostochastic*. If the desired matrix should be merely *unistochastic*, but not necessarily orthostochastic, the construction is even simpler. To this end let us consider the matrix

$$P^\alpha := U^\dagger D^\alpha U \quad (\text{C1})$$

where  $U$  is a unitary matrix diagonalizing  $P$ , where  $P$  is given by (B1), and  $D$  is a diagonal matrix,

$$D := \text{diag}(1, e^{2\pi i/N}, e^{4\pi i/N}, \dots, e^{2(N-1)\pi i/N}) \quad (\text{C2})$$

with the eigenvalues of  $P$  on the main diagonal. Hence, consequently

$$D^\alpha = \text{diag}(\Lambda_0, \Lambda_1, \dots, \Lambda_{N-1}) \quad (\text{C3})$$

where  $\Lambda_k := \exp(2k\alpha\pi i/N)$ ,  $k = 0, 1, \dots, N-1$ , are the eigenvalues of  $P^\alpha$ . Obviously  $P^\alpha$  is unitary and as a function of  $P$  can be written in the form  $P^\alpha := \sum_{j=0}^{N-1} a_j P^j$ , which gives for the eigenvalues

$$\Lambda_k = e^{2k\alpha\pi i/N} = \sum_{j=0}^{N-1} a_j \exp\left(\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N-1. \quad (\text{C4})$$

As previously we obtain the coefficients  $a_j$  by inverting the discrete Fourier transform

$$a_j = \frac{1}{N} \sum_{k=0}^{N-1} \Lambda_k \exp\left(-\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N-1. \quad (\text{C5})$$

The associated unistochastic matrix thus reads

$$B := \sum_{j=0}^{N-1} |a_j|^2 P^j \quad (\text{C6})$$

and has as the eigenvalues

$$\lambda_k = \sum_{j=0}^{N-1} |a_j|^2 \exp\left(\frac{2\pi i}{N}kj\right) \quad k = 0, 1, \dots, N-1 \quad (\text{C7})$$

i.e.

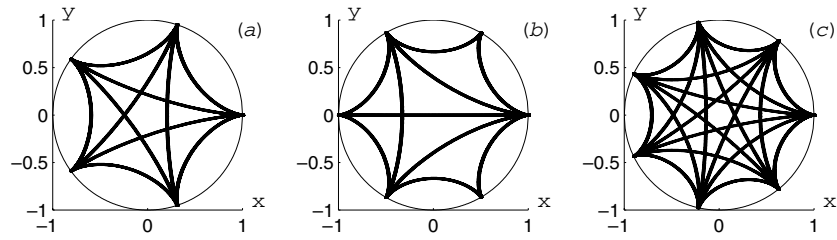
$$\begin{aligned} \lambda_k &= \frac{1}{N^2} \sum_{j=0}^{N-1} \sum_{l=0}^{N-1} \sum_{r=0}^{N-1} \Lambda_l \Lambda_r^* \exp\left(-\frac{2\pi i}{N}(l+r-k)j\right) \\ &= \frac{1}{N} \sum_{l=0}^{N-1} \sum_{r=0}^{N-1} \Lambda_l \Lambda_r^* \delta_{r,l-k} = \frac{1}{N} \sum_{l=0}^{N-1} \Lambda_l \Lambda_{l-k}^*, \end{aligned} \quad (\text{C8})$$

and hence

$$\lambda_1 = \frac{1}{N} \left( \Lambda_0 \Lambda_{N-1}^* + \sum_{l=1}^{N-1} \Lambda_l \Lambda_{l-1}^* \right) = \frac{1}{N} (e^{-2(N-1)\alpha\pi i/N} + (N-1)e^{2\alpha\pi i/N}) \quad (\text{C9})$$

which renders the  $N$ -hypocycloid for  $\alpha \in [0, N/2]$ . Similarly, the further eigenvalues  $\lambda_k$  generate the inner hypocycloids (e.g. 3-hypocycloid for  $N = 6$ , see figure 7), which proves proposition 3.

Observe that for  $N = 3$  the permutation matrices  $P$ ,  $P^2$  and  $P^3 = \mathbb{I}_3$  form an equilateral triangle (in the sense of the Hilbert–Schmidt distance, which is induced by the Frobenius



**Figure 7.** Spectra of a family of bistochastic matrices  $B^{(N,\alpha)}$  with  $\alpha \in [0, N/2]$  obtained by exponentiation of the permutation matrix  $P_N$  plotted for (a)  $N = 5$  (hypocycloids 5 and  $5/2$ ), (b)  $N = 6$  (hypocycloids 6,  $3 = 6/2$  and  $2 = 6/3$ ) and (c)  $N = 7$  (hypocycloids 7,  $7/2$  and  $7/3$ ).

norm of a matrix,  $\|P\| := \sqrt{PP^\dagger}$ . Comparing equations (C6) and (C7) with  $k = 1$  we see that both quantities have the same structure and the same dependence on the coefficients  $a_j$ , which are implicit functions of the parameter  $\alpha$ . Therefore, varying this parameter we obtain the very same curves in two entirely different spaces: the eigenvalue  $\lambda_1 = \lambda_1(\alpha)$  provides the 3-hypocycloid in the plane of complex spectra, while the family of unistochastic matrices  $B = B(\alpha)$  forms the same hypocycloid in the two-dimensional cross section of the four-dimensional body of  $N = 3$  bistochastic matrices determined by  $P, P^2$  and  $P^3$ .

**Appendix D. Interpolation between corners of two hypocycloids**

In this appendix we provide a discussion of a family of unistochastic matrices of size 4, the spectra of which are not contained in the sum of 2-, 3- and 4-hypocycloids. To find an interpolation between the corners of 3- and 4-hypocycloids, consider the orthogonal matrix  $\tilde{O}_{3,4}(\varphi) = O_4(\varphi)P_{(1234)}$ , as defined in section 4,

$$\tilde{O}_{3,4}(\varphi) := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \varphi & \sin \varphi \\ 0 & 0 & -\sin \varphi & \cos \varphi \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \varphi & \sin \varphi \\ 0 & 0 & -\sin \varphi & \cos \varphi \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{D1}$$

For  $\varphi$  varying in  $[0, \pi/2]$  this family interpolates between a four-element permutation  $P_{(1234)}$  and a matrix, the absolute values of which represent a three-element permutation  $P_{(124)(3)}$ . Thus the spectra of corresponding bistochastic matrices give an interpolation between the third and the fourth roots of identity. As shown in figure 4 this interpolation is located *outside* the hypocycloids  $H_3$  and  $H_4$ , so the support  $\Sigma_4^U$  is larger than their sum  $G_4$ . Repeating the argument with the multiplicative interpolation between any such matrix and the Fourier matrix  $F^{(4)}$ , we conclude that all points *inside* the set bounded by this interpolation belong to the support  $\Sigma_4^U$ . An analogous scheme allows us to find an  $(N - 1) \longleftrightarrow N$  interpolation. For example, the family of orthogonal matrices  $\tilde{O}_{4,5}(\phi) = O_5(\phi)P_{(12345)}$  of size 5 gives an interpolation between  $e^{\frac{2\pi i}{5}}$  and  $i = e^{\frac{2\pi i}{4}}$ .

To find the missing  $N = 4$  interpolation for the negative real part of the eigenvalues, consider a permutation of the orthogonal matrix which contains the block  $O_3$  responsible for the 3-hypocycloid,

$$\tilde{O}_{3,2} := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & c & a & b \\ 0 & b & c & a \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ a & 0 & c & b \\ c & 0 & b & a \\ b & 0 & a & c \end{bmatrix} \tag{D2}$$



where its elements  $a, b$  and  $c$  are functions of the angle  $\varphi$  as given in (4.11). Then the spectra of the corresponding orthostochastic matrices, obtained by squaring the elements of the above orthogonal matrices,

$$\tilde{B}_{3,4}(\varphi) := \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \cos^2 \varphi & \sin^2 \varphi \\ 0 & 0 & \sin^2 \varphi & \cos^2 \varphi \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad \tilde{B}_{3,2}(\varphi) := \begin{bmatrix} 0 & 1 & 0 & 0 \\ a^2 & 0 & c^2 & b^2 \\ c^2 & 0 & b^2 & a^2 \\ b^2 & 0 & a^2 & c^2 \end{bmatrix} \quad (\text{D3})$$

provide the required interpolations located outside hypocycloids  $H_3$  and  $H_4$  (see figures 4(b) and (d)). For larger dimensionality an analogous construction has to be performed to get the interpolations between the neighbouring roots of unity.

### Appendix E. Average traces of unistochastic matrices

To evaluate the average traces we rely on the results of Mello [54], who computed various averages,  $\langle \cdot \rangle$ , over the Haar measure on the unitary group  $U(N)$ . In particular, he found average values of the following quantities constructed of elements  $U_{ab}$  of a unitary matrix of size  $N$ :

$$Q_{b_1\beta_1, \dots, b_m\beta_m}^{a_1\alpha_1, \dots, a_k\alpha_k} := \langle (U_{b_1\beta_1} \cdots U_{b_m\beta_m})(U_{a_1\alpha_1} \cdots U_{a_k\alpha_k})^* \rangle. \quad (\text{E1})$$

Mean trace of a squared unistochastic matrix, defined by  $B_{ij} = |U_{ij}|^2$ , reads

$$\begin{aligned} t_{N,2} &:= \langle \text{Tr} B^2 \rangle_{\text{USE}} = \left\langle \sum_{i,k=1}^N (U_{ik} U_{ik}^*)(U_{ki} U_{ki}^*) \right\rangle_{U(N)} \\ &= \sum_{i,k=1}^N Q_{ik,ki}^{ik,ki} = N Q_{11,11}^{11,11} + N(N-1) Q_{12,21}^{12,21} \end{aligned} \quad (\text{E2})$$

since the symmetry of the problem allowed us to group together the terms according to the number of different indices. Using the results of Mello,  $Q_{11,11}^{11,11} = 2/(N(N+1))$  and  $Q_{12,21}^{12,21} = 1/(N(N+1))$ , we get  $t_{N,2} = (N+2)/(N+1)$ .

The mean trace of  $B^3$  reads

$$t_{N,3} := \langle \text{Tr} B^3 \rangle_{\text{USE}} = N Q_{11,11,11}^{11,11,11} + 3N(N-1) Q_{11,12,21}^{11,12,21} + N(N-1)(N-2) Q_{12,23,31}^{12,23,31}. \quad (\text{E3})$$

The data in Mello’s paper allow us to find  $Q_{11,11,11}^{11,11,11} = 6/[N(N+1)(N+2)]$ ,  $Q_{11,12,21}^{11,12,21} = 1/[(N+2)(N^2-1)]$  and  $Q_{12,23,31}^{12,23,31} = (N^2-2)/[(N(N^2-1)(N^2-4)]$ , where the last term (with three different indices) is present only for  $N \geq 3$ . Substituting these averages into (E3), we arrive at the result (4.21).

In the general case of arbitrary  $n$ , we may write a formula

$$t_{N,n} := \langle \text{Tr} B^n \rangle_{\text{USE}} = \sum_{i_1, \dots, i_n}^N Q_{i_1 i_2, i_2 i_3, \dots, i_{n-1} i_n, i_n i_1}^{i_1 i_2, i_2 i_3, \dots, i_{n-1} i_n, i_n i_1} \quad (\text{E4})$$

which is explicit, but not easy to simplify. An analogous computation for the ensemble of

symmetric unistochastic matrices may be based on the results of Brouwer and Beenakker [57], who computed the averages (E1) for COE.

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