Birkhoff’s Polytope and Unistochastic Matrices, N = 3 and N = 4

Ingemar Bengtsson1, Åsa Ericsson1, Marek Kuś2, Wojciech Tadej3, Karol Życzkowski1,4

1 Stockholm University, AlbaNova, Fysikum, 106 91 Stockholm, Sweden. E-mail: ingemar@physto.se; asae@physto.se
2 Centrum Fizyki Teoretycznej, Polska Akademia Nauk, Al. Lotników 32/44, 02–668 Warszawa, Poland. E-mail: marek@cft.edu.pl
3 Cardinal Stefan Wyszynski University, Warszawa, Poland. E-mail: wtadej@wp.pl
4 Instytut Fizyki im. Smoluchowskiego, Uniwersytet Jagielloński, ul. Reymonta 4, 30–059 Kraków, Poland. E-mail: karol@tatry.if.uj.edu.pl

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Abstract: The set of bistochastic or doubly stochastic N × N matrices is a convex set called Birkhoff’s polytope, which we describe in some detail. Our problem is to characterize the set of unistochastic matrices as a subset of Birkhoff’s polytope. For N = 3 we present fairly complete results. For N = 4 partial results are obtained. An interesting difference between the two cases is that there is a ball of unistochastic matrices around the van der Waerden matrix for N = 3, while this is not the case for N = 4.

1. Introduction

Unistochastic matrices arise in many different contexts including error correcting codes, quantum information theory and particle physics. To define them, we first recall that an N × N matrix B is said to be bistochastic if its matrix elements satisfy

i: \( B_{ij} \geq 0 \), \hspace{1cm} ii: \( \sum_i B_{ij} = 1 \), \hspace{1cm} iii: \( \sum_j B_{ij} = 1 \).

(1)

The set of bistochastic matrices is a convex polytope known as Birkhoff’s polytope.

One way of constructing a bistochastic matrix is to begin with a unitary matrix U and let

\[ B_{ij} = |U_{ij}|^2. \]

(2)

However, it is well-known [1] that not all bistochastic matrices arise in this way. If there is such a U, then we will call B unistochastic. If U is also real, that is orthogonal, then we call B orthostochastic. (Much of the mathematics literature uses the term orthostochastic to mean any matrix satisfying (2) and does not distinguish the subclass for which U is real. We will see later that the distinction is important.) In this paper, we consider the problem of characterizing the unistochastic subset of Birkhoff’s polytope.

Before summarizing our results, we mention some physical applications. In quantum mechanics, the transition probabilities associated with a finite basis form bistochastic...
matrices. In studies of the foundations of quantum theory, the attempt to build some group structure into these transition probabilities leads to the requirement that they form unistochastic matrices. A sample of the literature includes Landé [2], Rovelli [3] and Khrennikov [4].

In the attempt to formulate quantum mechanics on graphs (in the laboratory on thin strips of, say, gold film) the question of what Markov processes have quantum counterparts in the given setting again leads to unistochastic matrices [5–7]. In this connection studies of the spectra and entropies of unistochastic matrices chosen at random have been made [8].

In particle physics, a related question arises. In the theory of weak interactions one encounters the unitary Kobayashi-Maskawa matrices (one for quarks and one for neutrinos), and Jarlskog raised the question to what extent such a matrix can be parametrized by the easily measured moduli of its matrix elements. The physically interesting case here is $N = 3$ [9], and possibly also $N = 4$, should a fourth generation of quarks be discovered [10]. The question of determining $U$ from $B$ also arises in scattering theory, with no restriction on $N$ [11].

Our main result involves the van der Waerden matrix $J_N$, whose matrix elements satisfy $(J_N)_{ij} = \frac{1}{N}$. This matrix is unistochastic, and any corresponding unitary matrix is known as a complex Hadamard matrix. An example is the Fourier matrix, whose matrix elements are

$$U_{jk} = \frac{1}{\sqrt{N}} e^{2\pi i jk/N}, \quad 0 \leq j, k \leq N - 1.$$  

Here $q = e^{2\pi i/N}$ is a root of unity. Complex Hadamard matrices have a long history in mathematics [12–14], and have recently arisen in quantum information theory [15–17].

In this paper we study the set of unistochastic matrices, and the precise way in which it forms a subset of Birkhoff’s polytope. Our main result is that for $N = 4$ every neighborhood of the van der Waerden matrix contains matrices that are not unistochastic. This is in striking contrast with the $N = 3$ case for which $J_3$ is at the center of a ball of unistochastic matrices inside a star-shaped region bounded by the set of orthostochastic matrices.

This paper is organized as follows. In Sect. 2 we consider the set of all bistochastic matrices, and describe the cases $N = 3$ and $N = 4$ in detail ($N = 2$ is trivial). In Sect. 3 we discuss some generalities concerning unistochastic matrices, and then characterize the unistochastic subset in the case $N = 3$. Most of our results can be found elsewhere but, we believe, not in this coherent form. In Sect. 4 we consider $N = 4$, prove our main result, and relate some already known facts [10] to our explicit description of Birkhoff’s polytope. Section 5 summarises our conclusions. Some technical matters are found in three appendices.

2. Birkhoff’s Polytope

The set $B_N$ of bistochastic $N \times N$ matrices has $(N - 1)^2$ dimensions. To see this, note that the last row and the last column are fixed by the conditions that the row and column sums should equal one. The remaining $(N - 1)^2$ entries can be chosen freely, within limits. Birkhoff proved that $B_N$ is a convex polytope whose extreme points, or corners, are the $N!$ permutation matrices [18]. It is called Birkhoff’s polytope. All its corners are equivalent in the sense that they can be transformed into each other by means of orthogonal transformations. A bistochastic matrix belongs to the boundary of $B_N$ if and only if at least one of its entries is zero. The boundary consists of corners, edges, faces,