THE IMPORTANCE OF BEING UNISTOCHASTIC

Ingemar Bengtsson

Stockholm University, AlbaNova
Fysikum
S-106 91 Stockholm, Sweden

Abstract

A bistochastic matrix is a square matrix with positive entries such that rows and columns sum to unity. A unistochastic matrix is a bistochastic matrix whose matrix elements are the absolute values squared of a unitary matrix. We can now ask questions such as when a given bistochastic matrix is unistochastic. I review these questions: Why they are asked, why they are difficult to answer, and what is known about them.

1 The problem

There are some people that you have never heard of, but once you have met them for the first time they turn up everywhere. Unistochastic matrices are like that. First, some definitions: An $N \times N$ matrix $B$ is said to be bistochastic if its matrix elements obey

\begin{align}
&i: B_{ij} \geq 0 & ii: \sum_i B_{ij} = 1 & iii: \sum_j B_{ij} = 1 .
\end{align}

The first condition ensures that positive vectors are transformed to positive vectors. The second condition ensures that the sum of the components of the
vector remains invariant. A matrix obeying the first two conditions only is a 
**stochastic** matrix; if a discrete probability distribution is thought of as a vector \( \vec{p} \) then the vector \( \vec{q} = B\vec{p} \) is a probability distribution too. The third condition
ensures that the uniform distribution, a vector all of whose components are
equal, is transformed into itself. Hence a bistochastic matrix causes a kind of
contraction of the probability simplex with the uniform distribution as a fixed
point.

One way of obtaining a bistochastic matrix is to start with a unitary matrix
\( U \) and take the absolute value squared of its matrix elements,

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

(2)

If there exists such a \( U \) then \( B \) is said to be **unistochastic**. This raises two
mathematical questions:

**I**: Given a bistochastic matrix, is it unistochastic?

**II**: If so, to what extent is \( U \) determined by \( B \)?

My first task is clearly to convince you that these questions are interesting.

Indeed these questions occur in several approaches to quantum foundations.
An early example is that of Alfred Landé [1]. More recent examples include
those of Carlo Rovelli [2] and Andrei Khrennikov [3]. Roughly speaking the
reason is that one first argues that transition probabilities, suitably defined, form
bistochastic matrices. In attempting to build some group structure into these
transition probabilities one is then led to require that they form unistochastic
matrices, and the interference structure that is typical of quantum mechanics
follows. But here our questions I and II are clearly relevant.

Particle physicists form another set of people interested in unistochastic
matrices. Here question II is at the center of interest. Thus in the theory of
weak interactions we encounter the unitary Kobayashi–Maskawa matrix, and
Cecilia Jarlskog raised the question whether the difficult to measure phases in
this matrix—that contain CP–violating effects in the theory—can be obtained
by measuring the moduli of the matrix—that correspond to easily measured
decay rates. Up to “rephasing” (to be explained later) it turns out that \( B \)
determines \( U \) uniquely except for a discrete ambiguity for \( 3 \times 3 \) matrices [4],
while this is not so for \( 4 \times 4 \) [5]. As far as the KM matrix is concerned
\( N = 3 \) is the interesting case; \( N = 4 \) was studied just in case a fourth generation of
quarks should be discovered. (The same question occurs in scattering theory,
and there no restriction on \( N \) is imposed [6].)

Returning to quantum mechanics proper, there are various corners of quantum
information/computation theory where questions concerning unistochastic
matrices arise. My own interest came from an attempt to sharpen Schrödinger’s
mixture theorem (on the various ways that a given mixed state can be represented
as a mixture of pure states) [7]. Another example has to do with quantum
mechanics on graphs [8] [9]. In this connection studies of the spectra and
entropies of unistochastic matrices chosen at random have been made [10].
these applications question I comes to the fore again—in the second application rephrased as a question about what Markov processes that have a quantum counterpart in the given context. I will give further examples later when I have introduced a little more terminology.

Assuming that questions I and II are now on the table, let us begin by discussing the structure of the set $B_N$ of bistochastic $N \times N$ matrices. It is a convex polytope called Birkhoff’s polytope, a structure well known in the theory of linear programming. Its dimension is $(N - 1)^2$ and its corners are the $N!$ permutation matrices [11]. For $N = 2$ the set is just a line segment, while for $N = 3$ we have a four dimensional polytope with six corners. We can easily draw its graph, that is to say we draw all its corners and all its extremal edges. It turns out that all its edges are extremal, which is a rather exceptional property—in three dimensions only the simplex has this property.

For all $N$ Birkhoff’s polytope is centered at the van der Waerden matrix, all of whose matrix elements are equal. It is called that because van der Waerden made some conjecture about it. The van der Waerden matrix is always unistochastic. A corresponding unitary is the Fourier matrix, whose matrix elements are

$$U_{ij} = q^{ij}, \quad 0 \leq i, j \leq N - 1,$$

where $q = e^{2\pi i/N}$ is a root of unity. In general a unitary matrix giving rise to the van der Waerden matrix through eq. (2) is known as a complex Hadamard matrix. If it is real, it is known simply as an Hadamard matrix. The task of finding all real Hadamard matrices has occupied mathematicians since 1867 (when Sylvester first introduced them [12]); the problem is of considerable interest to computer scientists since Hadamard matrices are useful for constructing error correcting codes, and in other ways. Hadamard observed that they can exist only if $N = 2$ or $N = 4k$ and conjectured that they do exist in these dimensions [13]. His conjecture has proved a hard nut to crack [14]. In quantum information theory the restriction to real Hadamard matrices is not natural. An example of the usefulness of complex Hadamard matrices is provided by the fact that they can be used to construct bases of maximally entangled vectors. This in turn is an interesting problem because it is known that the set of maximally entangled bases is in one-to-one correspondence to the set of dense coding schemes, or equivalently teleportation schemes [15]. Let us see how the construction goes, choosing a Hilbert space of dimension $3 \times 3$ as an illustration. Choose a basis $|1\rangle, |2\rangle, |3\rangle$ in each factor Hilbert space. Write down the nine vectors

$$|1\rangle|1\rangle + |2\rangle|2\rangle + |3\rangle|3\rangle, \quad |1\rangle|1\rangle + q|2\rangle|2\rangle + q^2|3\rangle|3\rangle, \quad |1\rangle|1\rangle + q^2|2\rangle|2\rangle + q|3\rangle|3\rangle,$$

$$|1\rangle|2\rangle + |2\rangle|3\rangle + |3\rangle|1\rangle, \quad |1\rangle|2\rangle + q|2\rangle|3\rangle + q^2|3\rangle|1\rangle, \quad |1\rangle|2\rangle + q^2|2\rangle|3\rangle + q|3\rangle|1\rangle,$$

$$|1\rangle|3\rangle + |2\rangle|1\rangle + |3\rangle|2\rangle, \quad |1\rangle|3\rangle + q|2\rangle|1\rangle + q^2|3\rangle|2\rangle, \quad |1\rangle|3\rangle + q^2|2\rangle|1\rangle + q|3\rangle|2\rangle.$$
This is a generalization of the Bell basis in dimension $2 \times 2$, and all its members are maximally entangled by construction. That they form a basis is also evident. What we have done is to first write down a Latin square, and then to insert phases from the Fourier matrix to increase the number of orthogonal vectors from $3$ to $3 \times 3$. It is clear that the same construction will work whatever the value of $N$ we choose, and whatever Latin square and whatever complex Hadamard matrix we take. Thus the problem of classifying all dense coding schemes is at least as difficult as the problem of classifying all complex Hadamard matrices, plus the problem of classifying all Latin squares (a problem that we will not go into here).

The quantum optics community has also payed attention to complex Hadamard matrices [16]. They are sometimes referred to as Zeilinger matrices due to some scheme with symmetric multiports proposed by Zeilinger and collaborators [17].

2 Some modest results

Let us now take up question II in some earnest. It is clear that uniqueness cannot hold. Let $D_1$ and $D_2$ be diagonal unitary matrices. Then it is clear that $U$ and

$$U' = D_1 U D_2$$

(4)

will give rise to the same bistochastic matrix $B$ under eq. (2). The most we can hope for is a one-to-one correspondence between the set of unistochastic matrices and the double coset space

$$U(1) \times \ldots \times U(1) \setminus U(N)/U(1) \times \ldots \times U(1),$$

(5)

with $N$ $U(1)$ factors on the right and $N - 1$ factors on the left, say. The dimension of this space is the dimension of the set of unitaries minus $2N - 1$, that is $N^2 - (2N - 1) = (N - 1)^2$, which is the dimension of the set of bistochastic matrices. There is a slight problem in that the left action on the right coset space has fixed points, so our double coset space is not smooth. It is easy to locate the fixed points though, so that one can treat eq. (2) as a map between two smooth manifolds for most practical purposes. In practice the phase ambiguity is used to choose the first row and the first column to be real and positive. In this way we obtain what, in the particle physics community, is known as the set of dephased unitaries, and a preliminary conjecture might be that there is a one-to-one correspondence between the set of dephased unitaries and the set of bistochastic matrices. When $N = 2$ this conjecture is true.

For $N > 2$ it is false. For $N = 3$ a dephased unitary can be written as

$$\begin{bmatrix}
    r_{00} & r_{01} & \bullet \\
    r_{10} & r_{11} e^{i\phi_{11}} & \bullet \\
    r_{20} & r_{21} e^{i\phi_{21}} & \bullet
\end{bmatrix}.$$  

(6)
The moduli $r_{ij}$ are given (as square roots of matrix elements of a bistochastic matrix), and the question is whether one can find phases $\phi_{ij}$ such that this matrix is unitary. To do so it is enough to check that the first two columns are orthogonal; the last column will work out automatically which is why we do not write it explicitly. The problem is equivalent to that of choosing two angles so that three given lengths form a triangle. This may or may not be possible, depending on the lengths. (There are altogether six such “unitarity triangles” associated to our matrix. Interestingly they all have the same area [4].)

Since the answer to question I is sometimes yes, sometimes no, the question becomes that of understanding the set of unistochastic matrices as a subset of $B_3$. To do this we visualize the polytope, or at least we organize our impressions of it, with the observation that its $3 + 3$ corners form the vertices of two equilateral triangles that sit in two orthogonal 2-planes. Then we look at one of these triangles and see how the unistochastic subset sits in that triangle. Detailed study confirms the impression we get from this picture. The salient facts are that there is a ball of unistochastic matrices surrounding the van der Waerden matrix, and then there is a “spiky” structure which hits the boundary of the polytope in a two dimensional set. (Incidentally the unistochastic set has codimension 1 in the boundary for all $N$.) Technically the unistochastic set is star shaped and its relative volume is (numerically) close to 75 percent. Its boundary consists of orthostochastic matrices, that is bistochastic matrices for which the matrix $U$ can be taken to belong to the orthogonal group. The map from the set of dephased unitaries is generically two to one, so the answer to question II is that there is a discrete ambiguity.

The story for $N = 4$ is much richer. Birkhoff’s polytope is now nine dimensional and has 24 corners, which form altogether 6 regular tetrahedra. It is no longer true that all edges are extremal. The 2-dimensional faces consist of triangles and squares. (Incidentally this is true for any $N$ [18].) There are 18 squares altogether and their diagonals are precisely the edges of the regular tetrahedra. The polytope turns out to be organized around nine orthogonal hyperplanes, each containing the corners of four of the tetrahedra. Moreover each tetrahedron contains the normal vectors of three of the hyperplanes.

Questions I and II now become calculationally difficult to answer. Indeed very much so; an attempt to check whether a given bistochastic matrix is unistochastic using either a direct attack, or else some parametrization of unitary matrices, typically leads to algebraic equations of very high orders. So we are stuck with a difficult problem in algebraic geometry. It was pointed out already by Hadamard [13] that continuous ambiguities appear in the answer to question II. In fact the most general complex Hadamard matrix is (up to permutations of rows and columns)
\[
\frac{1}{2} \begin{bmatrix}
1 & 1 & 1 & 1 \\
1 & e^{i\phi} & -1 & -e^{i\phi} \\
1 & -1 & 1 & -1 \\
1 & -e^{i\phi} & -1 & e^{i\phi}
\end{bmatrix}.
\]

(7)

In a calculational tour de force, Auberson, Martin and Mennessier [5] were able to determine all bistochastic $4 \times 4$ matrices for which there are such continuous ambiguities in the answer to question II. Their occurrence clearly complicates matters. Detailed calculations shows that at a complex Hadamard matrix the tangent space of the set of dephased unitaries maps to one of the nine orthogonal hyperplanes around which the global structure of the polytope is organized: what we are looking at is a kind of nine dimensional snowflake where the center determines the periphery, and conversely. On the face of it there are two explanations for the degeneracy: Either we have the rather standard situation known from the “blow up of a point” in algebraic geometry, where the map from the set of dephased unitaries fails to be one-to-one at some isolated points, or, more dramatically, the van der Waerden matrix actually lies at the boundary of the unistochastic set. Unfortunately I do not know which is the case, but the evidence so far (from numerics and computer algebra) rather favours the latter explanation.\footnote{The latter explanation has since been proved to be the correct one [24].}

About higher dimensions not much is known, although we do have evidence that the set of unistochastic matrices always has the full dimension $(N - 1)^2$. For prime $N$ there is always a unistochastic ball around the van der Waerden matrix. When $N$ is not prime the situation is again unclear since the image of the tangent space at the Fourier matrix degenerates [19]. Complex Hadamard matrices have been looked for for modest values of $N$. There are some standard methods to produce them, such as using the character table of some finite group. (Choosing the cyclic group this gives exactly the Fourier matrix.) Further, typically non-equivalent, examples can be found if one first finds what is known as a bi-unimodular sequence, and then forms the circulant matrix of the sequence. The first examples of such sequences were found by Gauss, and all examples have been classified by Göran Björck up to $N = 8$ [20]. Examples of complex Hadamard matrices not coming from any of these two methods have been found for $N = 6$; continuous ambiguities appear when $N = 4, 6$ and $8$ while the solution for $N = 5$ is unique up to permutations of rows and columns. Continuous ambiguities also appear for some prime $N$, although Petrescu [21] has proved that the Fourier matrix is always an isolated point when $N$ is prime. For further information on this subject I recommend the papers by Haagerup [22] and by Dîta [23].
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