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NONSQUARE "DOUBLY STOCHASTIC" MATRICES

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An $n \times m$ non-negative matrix with uniform row sum m and column sum n is called a "doubly stochastic" matrix. When $n = m$, such a matrix is a scale multiple of a doubly stochastic matrix in its classical sense. Garrett Birkhoff proved a theorem characterizing all classical extremal doubly stochastic matrices as permutation matrices. We will discuss the characterization of the extremal matrices for nonsquare "doubly stochastic" matrices in the spirit of Birkhoff's theorem.

An $n \times m$ matrix $\mathbf{M} = (m_{ij})$ is called a *doubly stochastic* matrix (with uniform marginals) of size $n \times m$ if

$$\text{(uniform row marginals)} \qquad \sum_{j=1}^{m} m_{ij} = m \quad \text{for} \quad i = 1, 2, ..., n. \tag{1}$$

$$\text{(uniform column marginals)} \qquad \sum_{i=1}^{n} m_{ij} = n \quad \text{for} \quad j = 1, 2, ..., m. \tag{2}$$

$$\text{(positivity)} \qquad m_{ij} \geq 0 \quad \text{for} \quad i = 1, 2, ..., n \quad \text{and} \quad j = 1, 2, ..., m. \tag{3}$$

For example,

$$\mathbf{M}_1 = \begin{pmatrix} 1 & 3 & 0 & 0 \\ 1 & 0 & 3 & 0 \\ 1 & 0 & 0 & 3 \end{pmatrix} \quad \text{and} \quad \mathbf{M}_2 = \begin{pmatrix} 3 & 1 & 0 & 0 \\ 0 & 2 & 2 & 0 \\ 0 & 0 & 1 & 3 \end{pmatrix} \tag{4}$$

are two doubly stochastic matrices of size 3×4.

For integers $m, n \geq 1$, let $\mathcal{M}_{n \times m}$ denote the set of all doubly stochastic matrices of size $n \times m$. Then it is easy to see that $\mathcal{M}_{n \times m}$ is a convex set (of

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finite dimension). So

$\mathcal{M}_{n\times m}$ = the convex hull of extremal doubly stochastic matrices of size $n\times m$.

It is well known that in 1946 Garrett Birkhoff (Birkhoff (1946)) proved a theorem characterizing all extremal doubly stochastic *square* matrices. This can be stated in our notation as follows.

BIRKHOFF'S THEOREM: *If* $\mathbf{M} \in \mathcal{M}_{n\times n}$, *then* $\mathbf{M}$ *is extremal if and only if* $\frac{1}{n}\mathbf{M}$ *is a permutation matrix.*

We use the following equivalence relation:

DEFINITION. Two matrices of the same size are called equivalent if one can be transformed into the other by rearranging rows and columns.

Using this equivalence relation, we have

BIRKHOFF'S THEOREM RESTATED: *An* $n \times n$ *doubly stochastic matrix is extremal if and only if it is equivalent to the identity matrix times the scalar* n.

It is in the spirit of this form of Birkhoff's theorem that we want to characterize all extremal doubly stochastic matrices in $\mathcal{M}_{n\times m}$.

We remark that other types of characterization theorems are known. For example, it is shown in Li, Mikusiński, and Taylor (1997) that if we regard a matrix as a function on the set of its indices, then the uniqueness of the support of a doubly stochastic matrix is equivalent to the extremality of that matrix. A characterization in terms of graph theory is given in Balinski and Rispoli (1993) and Brualdi (1976). Another set of characterizations using submatrices appears in Jurkat and Ryser (1967).

Our approach is different in that we use a canonical representation of a matrix to check its extremality.

Some other references to extremal points and faces of polyhedra of doubly stochastic matrices are Brualdi and Gibson (1977), Gibson (1976), and Grzaślewicz (1985). The problem of the description of extremal infinite doubly stochastic matrices with given marginals was considered in Denny (1980), Grzaślewicz (1987), Isbel (1962), Kendall (1960), Letac (1966), and Mukerjee (1985). In the case of doubly stochastic measures, a functional analytic characterization of an extremal measure μ in terms of subspaces of $L_1(\mu)$ was given in Douglas (1964) and Lindenstrauss (1965).

From now on we assume $m \geq n$. We start with some simple results.

PROPOSITION 1. *If* $\mathbf{M} \in \mathcal{M}_{n\times m}$, *(where* $m \geq n$*) then the following hold:*

(i) Each column contains at least one positive entry.

(ii) Each row contains at least $\lceil m/n \rceil$ positive entries, where $\lceil x \rceil$ denotes the smallest integer not less than x.

If, in addition, M *is extremal, then*

(iii) All entries of M *are integers.*

PROOF. Assertions (i) and (ii) are immediate consequences of the definition of $\mathcal{M}_{n\times m}$ (cf. (1)-(3)). Assertion (iii) follows from Jurkat and Ryser (1967), Theorem 4.1, and the fact that in our case the row sum vector is $(m, m, ..., m) \in R^n$ and the column sum vector is $(n, n, ..., n) \in R^m$. ∎

REMARK. A more direct proof of assertion (iii) in Proposition 1 is to show that if there is a non-integer entry, then we can find a "cycle" (see Proposition 2 below) of non-integer entries, which contradicts the extremality of M.

The next result says that a matrix is extremal if and only if there is no "cycle" in its support. By a "cycle" we mean a sequence of "cells" or "positions" in the matrix of the form

$$(i_0, j_0),\ (i_1, j_0),\ (i_1, j_1),\ (i_2, j_1),\ (i_2, j_2), \cdots, (i_k, j_k), (i_0, j_k).$$

It may be visualized as a sequence of moves, alternately vertical and horizontal, from one cell of the support to another which ultimately returns to its starting point. Here is an example of a matrix whose support contains a cycle, and therefore it is not extremal:

$$\mathbf{M}_3 = \begin{pmatrix} 0 & \bullet & 0 & \bullet \\ \bullet & 0 & \bullet & \bullet \\ \bullet & \bullet & 0 & 0 \end{pmatrix},$$

where each '$\bullet$' indicates a positive entry. The cycle in this case may be taken to be

$$(2,1),\ (3,1),\ (3,2),\ (1,2),\ (1,4),\ (2,4).$$

PROPOSITION 2. *If* M$\in \mathcal{M}_{n\times m}$*, then* M *is extremal if and only if it is impossible to find distinct row indices $\{i_1, i_2, ..., i_p\}$ and distinct column indices $\{j_1, j_2, ..., j_p\}$ such that all entries at the following positions are positive:*

$$(i_q, j_q),\ q = 1, 2, ..., p;\ \ (i_q, j_{q+1}),\ q = 1, 2, ..., p-1;\ \ (i_p, j_1). \tag{5}$$

PROOF. Assume that there exist row indices $\{i_1, i_2, ..., i_p\}$ and column indices $\{j_1, j_2, ..., j_p\}$ such that all entries at the positions given in (5) are positive. Let $m_0 := \min(\{m_{i_q j_q} : q = 1, 2, ..., p\} \cup \{m_{i_q j_{q+1}} : q = 1, 2, ..., p -$

$1\} \cup \{m_{i_p,j_1}\})$. Then $m_0 > 0$. Set $m'_{ij} := m_{ij}$ if (i,j) is not one of the positions given in (5),

$$m'_{i_q,j_q} := m_{i_q,j_q} - m_0, \ q = 1,2,...,p$$

and

$$m'_{i_q,j_{q+1}} := m_{i_q,j_{q+1}} + m_0, \ q = 1,2,...,p-1; \ m'_{i_p,j_1} := m_{i_p,j_1} + m_0.$$

Then $M' := (m'_{ij}) \in \mathcal{M}_{n\times m}$, the support of $\mathbf{M}'$ is contained in the support of $\mathbf{M}$, and $M' \neq M$, which implies $\mathbf{M}$ is not extremal (see [14, Theorem 1]).

Now, assume $\mathbf{M}$ is not extremal. Then $\mathbf{M} = a\mathbf{A} + b\mathbf{B}$, where $a + b = 1, a > 0, b > 0$, $\mathbf{A}$ and $\mathbf{B} \in \mathcal{M}_{n\times m}$, and $\mathbf{A} \neq \mathbf{B}$. Now, $\mathbf{M} - \mathbf{A} = b(\mathbf{B} - \mathbf{A}) \neq \mathbf{0}$ has zero marginals. Note also that the positions of nonzero entries of $\mathbf{M} - \mathbf{A}$ are contained in the support of $\mathbf{M}$. We now demonstrate how to find a "cycle" in $\mathbf{M}$. Pick a positive entry in $\mathbf{M}-\mathbf{A}$, say at (i_1, j_1), then in the i_1-th row, there is a negative entry, say at (i_1, j_2); then in the j_2-th column, there is a positive entry, say at (i_2, j_2). By continuing to pick positive entries in the columns then negative entries in the rows alternatively, eventually we will arrive at an entry we have already picked up (since there are only finite number of nonzero entries in $\mathbf{M} - \mathbf{A}$); when this happens, we find a cycle in the support of $\mathbf{M}$. ∎

Proposition 2 is a special case of the general property of extremality (see, for example, Brualdi (1976) and Li, Mikusiński, Sherwood, and Taylor (1997)).

PROPOSITION 3. *If* $\mathbf{M} \in \mathcal{M}_{n\times m}$ *and each row of* $\mathbf{M}$ *contains exactly* $\lceil m/n \rceil$ *positive elements, then* $\mathbf{M}$ *is extremal.*

PROOF. Assume that $\mathbf{M} \in \mathcal{M}_{n\times m}$ and each row of $\mathbf{M}$ contains exactly $\lceil m/n \rceil$ positive elements but $\mathbf{M}$ is not extremal. Then, from Proposition 2, there exist distinct row indices $\{i_1, ..., i_p\}$ and distinct column indices $\{j_1, ..., j_p\}$ such that all entries of $\mathbf{M}$ at positions given by (5) are positive.

Let $k := \lceil \frac{m}{n} \rceil - 1$. From (1), we have

$$pm = \sum_{i=i_1,...,i_p} \sum_{j=1}^{m} m_{ij}.$$

Since each row has $k+1$ positive entries, there are exactly $(k+1)p$ positive entries in $\{m_{ij}\}_{i=i_1,i_2,...,i_p;\ j=1,2,...,m}$. Since these $(k+1)p$ positive entries include all positions given by (5), there are at least p columns containing (at least) two of these positive entries. So, at most $(k-1)p$ additional columns of $\mathbf{M}$ contain the rest of these $(k+1)p - 2p = (k-1)p$ positive entries. Thus, the $(k+1)p$ positive entries are contained in at most $p + (k-1)p$ columns of

M. So, from (2) and (3) we have

$$\sum_{i=i_1,\ldots,i_p} \sum_{j=1}^{m} m_{ij} \leq [p+(k-1)p]n = kpn.$$

Therefore, $pm \leq kpn$ or $\frac{m}{n} \leq \lceil \frac{m}{n} \rceil - 1$, which is impossible. ∎

When $n|m$, we can characterize the extremal matrices as follows.

PROPOSITION 4. *If $m = kn$, then all extremal elements of $\mathcal{M}_{n\times m}$ are equivalent to the following "block diagonal matrix":*

$$\begin{pmatrix} n & n & \ldots & n & & & & & & & & \\ & & & & n & n & \ldots & n & & & & \\ & & & & & & & & \ddots & & & \\ & & & & & & & & & n & n & \ldots & n \end{pmatrix}.$$

The proof of this result will be given at the end of the paper as a consequence of our main result, Theorem 5. Proposition 4 tells us that up to equivalence there is only one extremal matrix if $m = kn$. The situation becomes much more complicated when m is not a multiple of n. Note that $\mathbf{M}_1$ and $\mathbf{M}_2$ in (4) are both extremal in $\mathcal{M}_{3\times 4}$ but not equivalent. So, in general, there is more than one equivalence class of extremal matrices.

To see the kind of structure that can occur, look at the following examples.

Let $n = 7$ and $m = 16$ (note that $16 = 2 \times 7 + 2$),

$$\mathbf{M}_4 = \begin{pmatrix} 4 & 7 & 5 & & & & & & & & & & & & & \\ 3 & & & 7 & 3 & & & & & & & & 3 & & & \\ & & 2 & & & 7 & 7 & & & & & & & & & \\ & & & & 2 & & & 7 & 7 & & & & & & & \\ & & & & 2 & & & & & 7 & 7 & & & & & \\ & & & & & & & & & & & 5 & 4 & 7 & & \\ & & & & & & & & & & & 2 & & & 7 & 7 \end{pmatrix},$$

and

$$
\mathbf{M}_5 = \begin{pmatrix}
7 & 7 & 2 & & & & & & & & & & & & & \\
 & & 5 & 7 & 4 & & & & & & & & & & & \\
 & & & & 3 & 7 & 6 & & & & & & & & & \\
 & & & & & & 1 & 7 & 7 & 1 & & & & & & \\
 & & & & & & & & & 6 & 7 & 3 & & & & \\
 & & & & & & & & & & & 4 & 7 & 5 & & \\
 & & & & & & & & & & & & & 2 & 7 & 7
\end{pmatrix}.
$$

Matrices $\mathbf{M}_4$ and $\mathbf{M}_5$ are extremal in $\mathcal{M}_{7\times 16}$, but they are obviously not equivalent to each other.

We show next that, in general, we can transform matrices into some canonical form (like the form we used to express $\mathbf{M}_4$ and $\mathbf{M}_5$) from which we can easily see whether the matrices are extremal or not. To state our result, we need to describe the structure of a special class of matrices.

THE SIMPLE BLOCK: Each row of the block contains exactly $k+1$ positive entries. The first column of such a block contains all positive entries. This first column of positive entries is followed by l zero columns and l may be any integer greater than or equal to 0. After these zero columns, each column contains exactly one positive entry as indicated by

$$
\begin{pmatrix}
\bullet & \overbrace{0\ 0\ \cdots\ 0}^{l} & \overbrace{\bullet\ \bullet\ \cdots\ \bullet}^{k} & & & \\
\bullet & \overbrace{0\ 0\ \cdots\ 0}^{l} & & \overbrace{\bullet\ \bullet\ \cdots\ \bullet}^{k} & & \\
\vdots & & & & \ddots & \\
\bullet & \overbrace{0\ 0\ \cdots\ 0}^{l} & & & & \overbrace{\bullet\ \bullet\ \ldots\ \bullet}^{k}
\end{pmatrix} \tag{6}
$$

where each '$\bullet$' indicates a positive entry. We will refer to the blocks of k positive entries in each row as *diagonal elements*, and the number k as the *step length*.

The reader may notice that matrix $\mathbf{M}_4$ contains 4 simple blocks, and $\mathbf{M}_5$ contains 7 simple blocks.

TWO METHODS TO BUILD A MATRIX FROM THE SIMPLE BLOCKS: We present here two methods of putting simple blocks together. These are not the only ways in which they can be put together, but they will be of particular interest to us in what follows.

Method I (Without Jump): Given two blocks of form (6), we can construct a matrix by putting one block "above" the other so that their diagonal elements form a staircase pattern as the following figure indicates:

$$\begin{pmatrix} \bullet & 0\cdots 0 & \bullet\cdots\bullet & & & & \\ \vdots & & & \ddots & & & \\ \bullet & & & & \bullet\cdots\bullet & & \\ & & & \star 0 & \cdots 0 & \star\cdots\star & \\ & & & \vdots & & & \ddots \\ & & & \star & & & \star\cdots\star \end{pmatrix} \tag{7}$$

where '$\bullet$' and '$\star$' indicate positive entries in the two blocks respectively. In this situation, we will say the two blocks in (7) are connected together without jump.

Method II (With a Jump of Length $L+1$): Another way to construct a new matrix from two simple blocks is to put the two blocks at the diagonal position as follows:

$$\begin{pmatrix} \bullet & \overbrace{0\cdots 0}^{l} & \bullet\cdots\bullet & & & & & & \\ \vdots & & & \ddots & & & & & \\ \bullet & & & & \bullet\cdots\bullet & & & & \\ & & & & & \star & \overbrace{0\cdots 0}^{L} & \star\cdots\star & \\ & & & & & \vdots & & & \ddots \\ & & & & & \star & & & \star\cdots\star \end{pmatrix} \tag{8}$$

The number $L+1$ will be refered to as the *length* of the jump between the two blocks. So we will say the two blocks in (8) are connected together with a jump of length $L+1$.

These two methods can be used to construct matrices of interest from any given number of simple blocks of form (6).

With this terminology, we can state our main result.

THEOREM 5. *Assume* $\mathbf{M} \in \mathcal{M}_{n\times m}$ *is extremal and* $m = kn + r, 0 < r \leq n$.

Then $\mathbf{M}$ *is equivalent to the sum of two matrices* $\mathbf{M}_B$ *and* $\mathbf{M}_R$,

$$\mathbf{M}_B = \begin{pmatrix} B_1 & 0 & \cdots & 0 \\ 0 & B_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & B_r \end{pmatrix} \quad \text{and} \quad \mathbf{M}_R = \begin{pmatrix} 0 & R_{12} & \cdots & R_{1r} \\ 0 & 0 & \cdots & R_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

where the blocks in the two matrices are associated with the same row and column partitions, such that

(i) *each* B_i *is built from simple blocks using only method I (with step length* k*) each column of* B_i *has at least one positive entry;*

(ii) $\mathbf{M}_R$ *is a non-negative matrix with at most* $r-1$ *positive entries.*

Proof. We first show that matrix $\mathbf{M}$ can be transformed to an equivalent matrix of block upper triangular form

$$\begin{pmatrix} B_1 & R_{12} & \cdots & R_{1r} \\ 0 & B_2 & \cdots & R_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & B_r \end{pmatrix},$$

where each B_i is built from a number of simple blocks obtained by Method I (with step length k), each column of B_i has at least one positive entry, and each R_{ij} is a nonnegative matrix.

To ensure the following transformation can be carried out, we need only the following two properties of $\mathbf{M}$:

Property 1. Each row has at least $k+1$ positive entries.

Property 2. There is no cycle of positive entries in the matrix.

We note that these properties are verified in Propositions 1 and 2.

Now, we describe the transformation. We start by rearranging the rows of $\mathbf{M}$ so that, in the first column of $\mathbf{M}$, the positive entries are all above the zero entries. Assume there are s such positive entries. Next, we work with the first s rows of $\mathbf{M}$. In each of the first s rows of $\mathbf{M}$, there are at least k additional positive entries (by Property 1). These additional positive entries in different rows of the first s rows of $\mathbf{M}$ cannot share a column, otherwise a cycle of positive entries can be formed, contradicting Property 2. Therefore, we can interchange between columns 2 through m of $\mathbf{M}$ so that in rows 1 through s and columns 1 through $ks+1$ of $\mathbf{M}$ we obtain a simple block (with step length k). To initiate the second round of transformation, we concentrate on the submatrix $\mathbf{M}_1$ formed by rows $s+1$ to n and columns 2 to m of $\mathbf{M}$, and find the first nonzero column of $\mathbf{M}_1$. By rearranging the rows of $\mathbf{M}_1$ we can move up all rows with a positive entry in this column of $\mathbf{M}_1$ so that, in this column of $\mathbf{M}_1$, the positive entries are all above the zero entries. Note that Property 2 guarantees that there are at least k additional positive entries in these rows and from columns $ks+2$ to m of $\mathbf{M}$. So, as before, we can obtain a simple block (with step length k) in $\mathbf{M}_1$. Continue in this fashion until the process stops. (This will happen since there are only finitely many rows in $\mathbf{M}$.) Finally, by grouping neighboring simple blocks without jumps together we can form blocks B_i. Assume there are t such B_i blocks. Then $0 < t \leq n$. If B_i is of size $n_i \times m_i$, then $m_i = kn_i + 1$. Since $n = \sum_{i=1}^{t} n_i$ and $m = \sum_{i=1}^{t} m_i$, $m = \sum_{i=1}^{t}(kn_i + 1) = kn + t$. But $m = kn + r \quad (0 < r \leq n)$, so, $t = r$, or, in other words, there must be r such B_i blocks. Now, we see that $\mathbf{M}$ is transformed into the form as described at the beginning of the proof. So we have established (i).

Next, we verify (ii). Note that each R_{ij} can have at most one positive entry since otherwise a cycle of positive entries can be found in $\mathbf{M}$. Also, we claim that among the $r(r-1)/2$ matrices R_{ij} there are at most $r-1$ nonzero matrices. To prove this claim, we shall use the language of graph theory: We take the blocks B_i as the node set and two nodes B_i and B_j are connected by an edge if R_{ij} has a positive entry, then we get a graph. When two nodes B_i and B_j are connected, their positive entries are connected in the sense that any two positive entries can be taken as end points of a path (of horizontal and vertical lines) through only positive entries in the two blocks and R_{ij}. It is easy to see that when B_i and B_j are connected and B_j and B_k are also connected, the positive entries in B_i and B_k can also be connected (through positive entries in B_i, B_j, B_k, R_{ij} and R_{jk}). Therefore, whenever a set of nodes B_i are connected to form a cycle in the graph, there is a cycle of positive entries formed by the positive entries in these blocks. Since $\mathbf{M}$ is extremal, there must be no cycle of positive entries. So, the graph formed by the blocks B_i must be a forest (of trees). This is the case only if the number of the edges is (strictly) less than the number of the nodes (which is r), in other words, the number of nonzero matrices among R_{ij} must be less than or equal to $r-1$. ∎

Remark. Consider, for example, the matrix $\mathbf{M}_4$. Here we can take

$$\mathbf{M}_B = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix},$$

where

$$\mathbf{B}_1 = \begin{pmatrix} 4 & 7 & 5 & & & & & & & & \\ 3 & & & 7 & 3 & & & & & & \\ & & 2 & & & 7 & 7 & & & & \\ & & & & 2 & & & 7 & 7 & & \\ & & & & 2 & & & & & 7 & 7 \end{pmatrix} \text{ and } \mathbf{B}_2 = \begin{pmatrix} 5 & 4 & 7 & & \\ 2 & & & 7 & 7 \end{pmatrix}.$$

Using Theorem 5, we can prove the following.

PROPOSITION 6. *Suppose $m = kn + 1$ and $\mathbf{M} \in \mathcal{M}_{n \times m}$. Then $\mathbf{M}$ is extremal if and only if each row of $\mathbf{M}$ contains exactly $k+1$ positive entries.*

PROOF. The sufficiency is implied by Proposition 3. We now prove the necessity. Assume that $\mathbf{M}$ is extremal. By Theorem 5, $\mathbf{M}$ is equivalent to $\mathbf{M}_B + \mathbf{M}_R$. Since $r = 1$, so $\mathbf{M}_R = 0$. Thus $\mathbf{M} = \mathbf{M}_B$ and each row has exactly $k+1$ positive entries. ∎

PROOF OF PROPOSITION 4. By Theorem 5, $\mathbf{M}$ is equivalent to $\mathbf{M}_B + \mathbf{M}_R$ where each B_i in $\mathbf{M}_B$ is of size $1 \times k$ (k in Theorem 5 is $m/n - 1$ now). It is easy to see (by (2)) that $B_1 = (n, ..., n) \in R^k$. Then the first row of $\mathbf{M}_R$ must be zero because of (1). From this we have (by (2)) that $B_2 = (n, ...n) \in R^k$, and so the second row of $\mathbf{M}_R$ is also zero. Continuing in this fashion, we get that $\mathbf{M}_R = 0$ and

$$\mathbf{M} = \mathbf{M}_B = \begin{pmatrix} n \; n \; \dots \; n & & & \\ & n \; n \; \dots \; n & & \\ & & \ddots & \\ & & & n \; n \; \dots \; n \end{pmatrix}.$$

This completes the proof. ∎

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