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NOTES ON THE BIRKHOFF ALGORITHM FOR DOUBLY STOCHASTIC MATRICES

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ABSTRACT. The purpose of this note is to tie together some results concerning doubly stochastic matrices and their representations as convex combinations of permutation matrices.

Let Ω_n denote the set of $n\times n$ *doubly stochastic* matrices. Thus an $n\times n$ matrix $S=[s_{ij}]$ belongs to Ω_n provided $s_{ij}\geq 0$ $(i,j=1,\ldots,n)$, and the sum of the entries in each row and in each column of S equals one. It is readily verified that Ω_n is a convex polytope in Euclidean n^2-space, and it was shown in [8] that Ω_n has dimension n^2-2n+1. Birkhoff [1; 10, p. 58] proved that the extreme points of Ω_n are the $n\times n$ permutation matrices, and in doing so gave an algorithm for writing a doubly stochastic matrix as a convex combination of permutation matrices.

Let $A=[a_{ij}]$ be an $n\times n$ matrix of 0's and 1's such that for each (e,f) with $a_{ef}=1$, there is a permutation matrix $P=[p_{ij}]$ where $p_{ef}=1$ and $P\leq A$ (the order relation is entrywise). Then A is said to have *total support.* It was proved in [3] that the faces of Ω_n are in one-to-one correspondence with the $n\times n$ matrices A of 0's and 1's with total support; the face of Ω_n associated with A is

$$\mathscr{F}(A)=\{S\in\Omega_n : S\leq A\}.$$

If A has total support, then there is a largest integer $k\geq 1$ such that after reordering rows and columns, A is a direct sum $A_1\oplus\cdots\oplus A_k$ where $A_1,\ldots,A_k$ have total support. Since k is maximum $A_1,\ldots,A_k$ cannot be decomposed further into direct sums and are called the *fully indecomposable components* of A. It was proved in [3] by an elementary combinatorial argument that

$$\dim\mathscr{F}(A)=\sigma(A)-2n+k$$

where $\sigma(A)$ is the number of positive entries of A. It now follows from the

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classical theorem of Caratheodory [5] that every matrix in $\mathcal{F}(A)$ can be written as a convex combination of no more than $\sigma(A)-2n+k+1$ permutation matrices.

Let $S=[s_{ij}]\in\Omega_n$ and let $S_{(0,1)}$ be the matrix obtained from S by replacing each positive entry with a one. Thus $\mathcal{F}(S_{(0,1)})$ is the smallest face of Ω_n containing S. The *Birkhoff algorithm* for expressing S as a convex combination of permutation matrices proceeds as follows. Choose a smallest positive entry $c_1=s_{kl}$ of S. Then there exists a permutation matrix $P_1=[p_{ij}]$ such that $p_{kl}=1$ and $P_1\le S_{(0,1)}$. The matrix $S_1=S-c_1P_1$ is a nonnegative matrix having at least one more zero entry than S. We repeat with S_1 replacing S (the matrix S_1, if not the zero matrix, can be normalized to a doubly stochastic matrix if desired by multiplying by $1/(1-c_1)$), and continue until the zero matrix is obtained. We shall relax this algorithm somewhat by reversing the order of its two major components. Namely, we first choose a permutation matrix $P_1\le S_{(0,1)}$ and then choose the smallest (positive) entry in those positions of S corresponding to the 1's of P. The matrix $S_1=S-c_1P_1$ still has at least one more zero entry than S. We call any representation of S as a convex combination $c_1P_1+\cdots+c_tP_t$ of permutation matrices which is obtained in this way a *Birkhoff representation* of S.

How good is the Birkhoff algorithm? Good enough so that it expresses S as a convex combination of permutation matrices whose number does not exceed that which is guaranteed by Caratheodory's theorem:

(1) Birkhoff's algorithm expresses the doubly stochastic matrix S as a convex combination of no more than $\sigma(S_{(0,1)})-2n+k+1$ permutation matrices (where k is the number of fully indecomposable components of $S_{(0,1)}$).

The property (1) above was first established by Johnson, Dulmage, and Mendelsohn [7]. Another proof has been given by Nishi [9]. An alternative, and perhaps more revealing, proof can be given using the property:

(2) Each step of Birkhoff's algorithm lowers by at least one the dimension of the smallest face of Ω_n containing the doubly stochastic matrix.

To verify (2), let S be an $n\times n$ doubly stochastic matrix. It suffices to assume that $S_{(0,1)}$ is fully indecomposable. Let $T=(1-c)^{-1}\,(S-cP)$ where $P\le S_{(0,1)}$ is a permutation matrix and c is the smallest positive entry of S at positions corresponding to the 1's of P. Then T is doubly stochastic and has at least one more zero entry than S. The matrix $T_{(0,1)}$ then has total support and at least one more zero entry than $S_{(0,1)}$. Suppose that $T_{(0,1)}$ has $p\ge 1$ fully indecomposable components. Then after reordering of rows and columns, $T_{(0,1)}=B_1\oplus\cdots\oplus B_p$ where $B_1,\ldots,B_p$ are fully indecomposable. Since $T_{(0,1)}\le S_{(0,1)}$

and $S_{(0,1)}$ is fully indecomposable, it follows that $\sigma(S_{(0,1)}) \geq \sigma(T_{(0,1)}) + p$. Hence

$$\begin{aligned}\dim \mathcal{F}(T_{(0,1)}) &= \sigma(T_{(0,1)}) - 2n + p \\ &\leq \sigma(S_{(0,1)}) - p - 2n + p \\ &\leq \dim \mathcal{F}(S_{(0,1)}) - 1.\end{aligned}$$

Property (1) is now a consequence of (2). For, if $S \in \Omega_n$ and $S_{(0,1)}$ has k fully indecomposable components, then $\dim \mathcal{F}(S_{(0,1)}) = \sigma(S_{(0,1)}) - 2n + k$. Hence after at most $\sigma(S_{(0,1)}) - 2n + k$ steps of the Birkhoff algorithm, the resulting doubly stochastic matrix lies in a face of Ω_n of dimension 0, that is, is a permutation matrix. It follows that S is then expressed as a convex combination of at most $\sigma(S_{(0,1)}) - 2n + k + 1$ permutation matrices.

A lower bound for the minimum number of permutation matrices in a representation of a doubly stochastic matrix as a convex combination of permutation matrices can be obtained as follows. Let $A = [a_{ij}]$ be an $n \times n$ matrix of 0's and 1's with total support. Let U be a set of positions of A such that $(k, l) \in U$ implies $a_{kl} = 1$. Then U is said to be *strongly stable* [2] provided each permutation matrix $P = [p_{ij}]$ with $P \leq A$ satisfies $p_{kl} = 1$ for at most one $(k, l) \in U$. Denote by $\alpha(A)$ the maximum cardinality of a strongly stable set of positions of A. In [2] it is shown that $\alpha(A) = \max \sigma(X)$ where the maximum is taken over all submatrices X of A such that the submatrix of A complementary to X (the one formed by the rows complementary to the rows in which X lies and the columns complementary to the columns in which X lies) is a $p \times (n-1-p)$ zero submatrix for some $p = 0, 1, \ldots, n-1$. In particular, $\alpha(A)$ is at least equal to the maximum number of 1's in a row (take $p = n-1$) and in a column (take $p = 0$) of A. The following property is immediate.

(3) The $n \times n$ doubly stochastic matrix S cannot be expressed as a convex combination of fewer than $\alpha(S_{(0,1)})$ permutation matrices. In particular, Birkhoff's algorithm expresses S as a convex combination of at least $\alpha(S_{(0,1)})$ permutation matrices.

In (1) and (3) are given upper and lower bounds for the number of steps required in any application of Birkhoff's algorithm to a doubly stochastic matrix. We shall show that in each case equality can always be obtained and in the following strong sense: no matter how Birkhoff's algorithm is carried out the number of permutation matrices achieves equality. Before doing so, we first illustrate the following property:

(4) The number of permutation matrices in a Birkhoff representation of a doubly stochastic matrix S need not be unique.

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Let S be the doubly stochastic matrix

$$\frac{1}{6}\begin{bmatrix} 1 & 4 & 0 & 1 \\ 2 & 1 & 3 & 0 \\ 2 & 1 & 1 & 2 \\ 1 & 0 & 2 & 3 \end{bmatrix}.$$

Then $S=\frac{1}{6}P_1+\frac{1}{6}P_2+\frac{1}{3}P_3+\frac{1}{3}P_4$ is a Birkhoff representation of S, where

$$P_1=\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad P_2=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$P_3=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad P_4=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Also $S=\frac{1}{6}Q_1+\frac{1}{6}Q_2+\frac{1}{6}Q_3+\frac{1}{6}Q_4+\frac{1}{3}Q_5$ is a Birkhoff representation of S where

$$Q_1=\begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad Q_2=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad Q_3=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$Q_4=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad Q_5=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Let A be an $n\times n$ matrix of 0's and 1's with total support. Then from the formula for $\alpha(A)$ it follows that the strong stability number $\alpha(A)$ of A satisfies $1\le\alpha(A)\le\lceil n/2\rceil\lceil(n+1)/2\rceil$. If $n\ge 2$ and A is fully indecomposable, then each row and column of A contains at least two 1's, so that $2\le\alpha(A)$.

(5) Let t be an integer with $1\le t\le\lceil n/2\rceil\lceil(n+1)/2\rceil$. Then there exists an $n\times n$ doubly stochastic matrix S such that $\alpha(S_{(0,1)})=t$ and each Birkhoff representation of S uses exactly t distinct permutation matrices.

If $t=1$, then in (5) we may take S to be an $n\times n$ permutation matrix. To complete the verification we let $t\ge 2$ and construct an $n\times n$ fully indecomposable matrix A of 0's and 1's with $\alpha(A)=t$ such that $\mathscr{F}(A)$ is a simplex of dimension $t-1$. It then follows that a doubly stochastic matrix S in the interior of $\mathscr{F}(A)$ (that is, $S_{(0,1)}=A$) requires exactly t distinct permutation matrices in each of its representations as a convex combination of permutation matrices.

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Let p and q be positive integers with $p+q=n-1$. Let E be the $(q+1)\times q$ vertex-edge incidence matrix of a tree and F the $(p+1)\times p$ vertex-edge incidence matrix of a tree. Let X be any $(q+1)\times(p+1)$ matrix of 0's and 1's such that the $n\times n$ matrix

$$A=\begin{bmatrix} X & E \\ F^t & 0 \end{bmatrix}$$

has at least two 1's in each row and column. Then it follows from results in [3] that A is fully indecomposable and $\mathcal{F}(A)$ is a simplex of dimension $\sigma(A)-2n+1=\sigma(X)-1$. Since $\alpha(A)\geq\sigma(X)$, it follows that $\alpha(A)=\sigma(X)$. Now choose $p=\lfloor (n-1)/2\rfloor$ and $q=\lfloor n/2\rfloor$, and choose E and F to be vertex-edge incidence matrices of paths whose initial and terminal vertices correspond, respectively, to the first and last row. Then all row and column sums of A will be at least 2 if the entries of X in positions $(1, 1)$ and $(q+1, p+1)$ equal one. Since $(q+1)\times(p+1)=\lceil n/2\rceil\lceil (n+1)/2\rceil$, the conclusion now follows.

To construct matrices for which equality occurs in (1), we first need to review some ideas. A fully indecomposable matrix A is called *nearly decomposable* provided each matrix obtained from A by replacing a 1 with 0 is not fully indecomposable (it could not even be of total support). Let A be an $n\times n$ nearly decomposable matrix of total support with $n\geq 2$. Then [6, see also 4] there exists an integer n_1 with $1\leq n_1\leq n-1$ and an $n_1\times n_1$ nearly decomposable matrix A_1 such that after reordering rows and columns, A has the form

$$\text{(6)}\qquad \left[\begin{array}{c|ccccc} A_1 & & & E & & \\ \hline & 1 & 0 & \cdots & 0 & 0 \\ & 1 & 1 & \cdots & 0 & 0 \\ F & \vdots & \vdots & & \vdots & \vdots \\ & 0 & 0 & \cdots & 1 & 0 \\ & 0 & 0 & \cdots & 1 & 1 \end{array}\right]$$

where all entries of E and F are zero except for the entry of each in the upper right corner. If $n_1>1$, a similar decomposition holds for A_1, and so on.

Associated with an $n\times n$ matrix $A=[a_{ij}]$ of 0's and 1's is a bipartite graph $BG(A)$ of $2n$ vertices $x_1,\ldots,x_n, y_1,\ldots,y_n$; there is an edge joining x_i and y_j if and only if $a_{ij}=1$ $(i, j=1,\ldots,n)$, and these are the only edges. Let A be fully indecomposable. By rearranging rows and columns, we may assume that $I_n\leq A$ where I_n is the $n\times n$ identity matrix. Since A is fully indecomposable, $BG(A)$ is connected. Hence there is a spanning tree of $BG(A)$ which has among its edges the n edges $[x_1, y_1],\ldots,[x_n, y_n]$ of $BG(A)$. This spanning tree is associated with an $n\times n$ matrix T of 0's and 1's where $I_n\leq T\leq A$. We call T a *tree matrix*; note that $\sigma(T)=2n-1$.

For $1 \le p, q \le n$, the $n \times n$ matrix $E = [e_{ij}]$ where $e_{pq} = 1$ and $e_{ij} = 0$ otherwise is denoted by E^n_{ij}.

(7) Let A be an $n \times n$ fully indecomposable matrix of 0's and 1's. Then there is a tree matrix T with $I_n \le T \le A$ such that the $p = \sigma(A) - 2n + 1$ positions of $A - T$ whose entries equal one can be ordered as $(i_1, j_1), \ldots, (i_p, j_p)$ where for $l = 1, \ldots, p$ there is a permutation matrix P_l whose (i_l, j_l) entry equals one and

$$P_l \le T + E^n_{i_1 j_1} + \cdots + E^n_{i_l j_l}.$$

We first verify (7) for nearly decomposable matrices by induction on n. The case $n = 1$ being trivial, we let $n \ge 2$. We may assume A has the form (6) where A_1 is an $n_1 \times n_1$ nearly decomposable matrix and $1 \le n_1 \le n - 1$. By induction there is a tree matrix T_1 with $I_{n_1} \le T_1 \le A_1$ such that the s positions of $A_1 - T_1$ with a nonzero entry can be ordered as $(i_1, j_1), \ldots, (i_s, j_s)$ where for $l = 1, \ldots, s$ there is a permutation matrix Q_l whose (i_l, j_l) entry is one and

$$Q_l \le T_1 + E_{i_1 j_1} + \cdots + E_{i_l j_l}.$$

Let

$$T = \left[\begin{array}{c|ccccc} T_1 & & & 0 & & \\ \hline & 1 & 0 & \cdots & 0 & 0 \\ & 1 & 1 & \cdots & 0 & 0 \\ F & \vdots & \vdots & & \vdots & \vdots \\ & 0 & 0 & \cdots & 1 & 0 \\ & 0 & 0 & \cdots & 1 & 1 \end{array}\right]$$

Then $I_n \le T \le A$ and T is a tree matrix. Since A is nearly decomposable (and hence fully indecomposable) there is a permutation matrix $P \le A$ whose $(1, n)$-entry equals one. It now follows easily that the ordering $(i_1, j_1), \ldots, (i_s, j_s), (1, n)$ of the positions of $A - T$ with a nonzero entry has the required properties; the required permutation matrices are $P_1 = Q_1 \oplus I_{n-n_1}, \ldots, P_s = Q_s \oplus I_{n-n_1}, P_{s+1} = P$. Thus (7) holds for nearly decomposable matrices. Now let B be an $n \times n$ fully indecomposable matrix which is not nearly decomposable. Then by replacing certain 1's with 0's, we arrive at a nearly decomposable matrix A with $A \le B$. Let T be a tree matrix with $I_n \le T \le A$ satisfying (7). Ordering the positions of $B - T$ with nonzero entries as $(i_1, j_1), \ldots, (i_p, j_p), (i_{p+1}, j_{p+1}), \ldots, (i_q, j_q)$ where $(i_{p+1}, j_{p+1}), \ldots, (i_q, j_q)$ are the positions of $B - A$ with a nonzero entry in any order, we complete the verification.

We now construct doubly stochastic matrices for which equality holds in (1).

(8) Let A be an $n\times n$ fully indecomposable matrix of 0's and 1's. Then in the notation of (7) the matrix

$$S=\frac{1}{2^{p+1}-1}(2^pI_n+2^{p-1}P_1+\cdots+2P_{p-1}+P_p)$$

is in the face $\mathcal{F}(A)$ of dimension $p=\sigma(A)-2n+1$. Every representation of S as a convex combination of permutation matrices requires at least $p+1$ distinct permutation matrices. Every Birkhoff representation of S requires exactly $p+1$ permutation matrices.

To verify (8) we argue with $S'=(2^{p+1}-1)S$ instead of S. Suppose S' is written as a nonnegative linear combination of t permutation matrices $Q_1,\ldots,Q_t$. At least one of the matrices $Q_1,\ldots,Q_t$ has a one in the (i_p,j_p)-position, and the sum of the coefficients of all such matrices is $b_p=1$. Hence at least one of the permutation matrices $Q_1,\ldots,Q_t$ has a zero in the (i_p,j_p)-position and a one in the (i_{p-1},j_{p-1})-position; the sum of the coefficients of all such matrices is b_{p-1} where $1\le b_{p-1}\le 2$. Since $b_p+b_{p-1}\le 3$, at least one of the permutation matrices $Q_1,\ldots,Q_t$ has a zero in positions (i_p,j_p), (i_{p-1},j_{p-1}), and a one in position (i_{p-2},j_{p-2}); the sum of the coefficients of all such matrices is b_{p-2} where $1\le b_{p-2}\le 2^2$. Continuing like this we see that $t\ge p+1$. Since $\dim\mathcal{F}(A)=p=\sigma(A)-2n+1$, it follows from (1) that each Birkhoff representation of S requires at most $p+1$ distinct permutation matrices and hence exactly $p+1$ distinct permutation matrices.

Let A be an $n\times n$ matrix of 0's and 1's of total support with k fully indecomposable components. Using (8) one can construct doubly stochastic matrices $S\in\mathcal{F}(A)$ whose Birkhoff representations require exactly $\dim\mathcal{F}(A)+1=\sigma(A)-2n+k+1$ distinct permutation matrices.

We conclude these notes with some questions. Let $m=n!$ Since the vertices of Ω_n are the $n\times n$ permutation matrices $P_1,\ldots,P_m$, the map

$$f:(c_1,\ldots,c_m)\to c_1P_1+\cdots+c_mP_m$$

from the $(m-1)$-dimensional simplex $\{(c_1,\ldots,c_m): c_i\ge 0, \sum_i c_i=1\}$ to Ω_n is a continuous surjection, and for each $S\in\Omega_n$, $f^{-1}(S)$ is a compact convex set. Each m-tuple in $f^{-1}(S)$ furnishes a representation of the doubly stochastic matrix S as a convex combination of permutation matrices. It is a fundamental and very difficult question to ask for the m-tuple in $f^{-1}(S)$ with the fewest number of positive coordinates, that is, for a representation of S as a convex combination of the smallest possible number $c(S)$ of distinct permutation matrices. The properties (1) and (3) furnish upper and lower bounds on $c(S)$. It seems unlikely that a Birkhoff representation always exists with $c(S)$ distinct permutation matrices, although we have not constructed an example to substantiate this. It is easy to see that a Birkhoff representation corresponds to an extreme point of the polytope $f^{-1}(S)$. Are there other extreme points? The answer most likely is in the affirmative; otherwise, there would have to be a Birkhoff representation of S with $c(S)$ permutation matrices.

Doubly stochastic matrices have been used as a basic data structure for storing and processing uncertain information in multisensor data correlation [12, 13]. In these papers, the *entropy* of an $n \times n$ doubly stochastic matrix S has been defined by

$$H(S) = \sup \{h(c_1, \ldots, c_m) : (c_1, \ldots, c_m) \in f^{-1}(S)\},$$

where $H(c_1, \ldots, c_m) = \sum_{i=1}^{m} -c_i \log c_i$, the entropy of the probability distribution $(c_1, \ldots, c_m)$. Thus the entropy of a permutation matrix is 0 and that of the $n \times n$ matrix J_n with each entry equal to $1/n$ is $\log n!$ The entropy of every other $n \times n$ doubly stochastic matrix S satisfies $0 \le H(S) \le \log n!$. An $n \times n$ doubly stochastic matrix S can be regarded as a probabilistic model of a bijection $h : X \to Y$ between two sets of n elements, a *fuzzy bijection*. The row sums of S being one means every element of X for sure goes someplace; the column sums of S being one means for sure every element of Y comes from someplace. Birkhoff's theorem then becomes: every fuzzy bijection is a convex combination of bijections. Since one interpretation of entropy of a probability distribution is that of a measure of uncertainty, the entropy of a fuzzy bijection (doubly stochastic matrix) can be interpreted as a measurement of the uncertainty concerning which bijection is involved. For a doubly stochastic matrix S, which representation as a convex combination of permutation matrices has entropy equal to $H(S)$? What is the largest entropy of a Birkhoff representation?

Finally we note that an extension of Birkhoff's algorithm to doubly stochastic matrices over more general number systems has been considered in [11].

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