The Minimum Coefficient of Ergodicity for a Markov Chain with a Given Directed Graph

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Abstract

Suppose that T is an $n \times n$ stochastic matrix, and denote its directed graph by $\mathcal{D}(T)$. The function $\tau(T) = \frac{1}{2}\max_{i,j=1,\ldots,n}\{||(e_i - e_j)^\top T||_1\}$ is known as a coefficient of ergodicity for T, and measures the rate at which the iterates of a Markov chain with transition matrix T converge to the stationary distribution vector. Many Markov chains are equipped with an underlying combinatorial structure that is described by a directed graph, and in view of that fact, we consider the following problem: given a directed graph D, find $\tau_{\min}(D) \equiv \min \tau(T)$, where the minimum is taken over all stochastic matrices T such that $\mathcal{D}(T)$ is a spanning subgraph of D.

In this paper, we characterise $\tau_{\min}(D)$ as the solution to a linear programming problem. We then go on to provide an upper bound on $\tau_{\min}(D)$ in terms of the maximum outdegree of D, and a lower bound on $\tau_{\min}(D)$ in terms of the maximum indegree of D, characterising the equality cases in both bounds. Connections are established between the equality case in the lower bound and certain balanced incomplete block designs.

Keywords: Stochastic matrix; Directed graph; Coefficient of ergodicity.
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1 Introduction and motivation

A square matrix T of order n is *stochastic* if it is entrywise nonnegative, and $T\mathbf{1}_n = \mathbf{1}_n$, where $\mathbf{1}_n$ denotes the all ones vector in $\mathbb{R}^n$. The class of stochastic matrices is

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much–studied, in large part because it is at the centre of the theory of discrete–time Markov chains on finite state space. If the Markov chain under consideration is time–homogeneous with transition matrix T, then the iterates of the chain, say $x(k), k = 0, 1, 2, \dots$ satisfy the relation $x(k)^\top = x(0)^\top T^k$, where $x(0)$ is an initial distribution vector that is nonnegative and has entries summing to 1.

Suppose that T is primitive; its *stationary distribution vector*, say w, is the left Perron vector of T normalised so that $w^\top \mathbf{1}_n = 1$. It then follows that $x(k) \to w$ as $k \to \infty$, regardless of the initial distribution vector $x(0)$. How quickly do the iterates of such a Markov chain converge to w? Since the Markov chain is a realisation of the power method with iteration matrix T, it is clear that the asymptotic rate of convergence is governed by the moduli of the non–Perron eigenvalues of T. However, there are other measures of the rate of convergence that are considered in the literature on Markov chains. In this paper we focus on the following quantity, which is known as a *coefficient of ergodicity*: given an $n \times n$ stochastic matrix T, define the function $\tau(T)$ via

$$\tau(T) = \max_{x^\top \mathbf{1}=0, ||x||_1=1} ||x^\top T||_1. \qquad (1)$$

(Here $||\cdot||_1$ denotes the ℓ_1 norm of a row or column vector.) We note in passing that there are other functions that serve as coefficients of ergodicity; see [5] for a survey on that topic. A result of Seneta [10, section 2.5] shows that $\tau(T)$ can be computed explicitly as

$$\tau(T) = \frac{1}{2} \max_{i,j=1,\dots,n} ||(e_i - e_j)^\top T||_1, \qquad (2)$$

where for each $k = 1, \dots, n$, e_k denotes the k–th standard unit basis vector in $\mathbb{R}^n$. From (2) we find that $\tau(PTQ) = \tau(T)$ for any $n \times n$ permutation matrices P and Q. Further, it follows readily from (2) that $\tau(T) \le 1$ for any stochastic matrix T, and that $\tau(T) < 1$ if and only if T is *scrambling* – that is, for each pair of rows of T, there is a position in which both rows have a positive entry.

Suppose that we have a nonnegative vector x whose entries sum to 1; from (1), we see that $||x^\top T - w^\top||_1 = ||(x - w)^\top T||_1 \le \tau(T)||x^\top - w^\top||_1$. In particular, if $x \ne w$, we have $\frac{||x^\top T - w^\top||_1}{||x^\top - w^\top||_1} \le \tau(T)$. Further, if i and j are indices such that $\frac{1}{2}||(e_i - e_j)^\top T||_1 = \tau(T)$, and if we have $y = w + \epsilon(e_i - e_j)$ for a sufficiently small ϵ, then y is a positive vector and

$$\frac{||y^\top T - w^\top||_1}{||y^\top - w^\top||_1} = \frac{||\epsilon(e_i - e_j)^\top T||_1}{||\epsilon(e_i - e_j)||_1} = \frac{1}{2}||(e_i - e_j)^\top T||_1 = \tau(T).$$

From these two observations, we find that

$$\tau(T) = \max\left\{ \frac{||x^\top T - w^\top||_1}{||x^\top - w^\top||_1} \middle| x \text{ is a positive vector}, x^\top \mathbf{1}_n = 1, x \ne w \right\}.$$

Consequently $\tau(T)$ provides precise information on the relative improvement in the distance to w that can be guaranteed to be observed in a single step of the Markov chain associated with T. Hence the function τ can be thought of as another measure of the rate of convergence of the iterates of a Markov chain.

The function $\tau(T)$ also serves as an upper bound on the modulus of any non–Perron eigenvalue of T (see [10]), and so can be used as a proxy for the asymptotic rate of convergence of the Markov chain in situations where the spectrum of T is difficult to compute or analyse. Further, in [11], Seneta shows how $\tau(T)$ can play a role in measuring the conditioning of the stationary distribution when T is perturbed; in particular, small values of $\tau(T)$ correspond to stationary distribution vectors that are well conditioned. Finally, we note that the function τ plays a central role in understanding the asymptotic behaviour of Markov chains that are time inhomogeneous (see [10, section 4.3]). The utility of τ in the context of inhomogeneous Markov chains follows in part from the fact (readily deduced from (1)) that we have $\tau(T_1T_2) \leq \tau(T_1)\tau(T_2)$ whenever T_1 and T_2 are stochastic matrices of the same order.

Given a stochastic matrix T of order n, the *directed graph of* T, which we denote by $\mathcal{D}(T)$, has vertices labelled $1, \ldots, n$, with an arc $i \rightarrow j$ for all ordered pairs (i, j) such that $t_{i,j} > 0$. The directed graph of T carries important information; for example the irreducibility or primitivity of T, as well as the classification of the states of the corresponding Markov chain as either essential or transient, can all be determined from this directed graph. In some applications of Markov chains (for instance, in the traffic and emission models of [3] and [4]), the directed graph of the corresponding transition matrix is specified by the phenomenon being modelled. In view of this fact, there is merit in bringing the directed graph into consideration when analysing the properties of stochastic matrices. Existing research in this direction includes: a bound on the modulus of the non–Perron eigenvalues of T in terms of the length of the shortest cycle in $\mathcal{D}(T)$ ([6]); computation of the smallest possible Kemeny constant over the class of stochastic matrices T such that $\mathcal{D}(T)$ is subordinate to a given directed graph ([7]); and minimisation of the largest entry in the stationary distribution, again when $\mathcal{D}(T)$ is subordinate to a given directed graph ([8]). In this paper, we continue this line of investigation by addressing the following problem. Let D be a directed graph on n vertices such that each vertex has outdegree at least 1; find $\min\{\tau(T)|T$ is stochastic and $\mathcal{D}(T)$ is a spanning subgraph of $D\}$. (Evidently this question is only interesting if the class of matrices over which we minimise τ includes at least one scrambling stochastic matrix.)

In fact we will focus our attention on a slightly larger class of matrices, namely the rectangular nonnegative matrices with all row sums equal to 1. If M is $n \times m$ and nonnegative with $M\mathbf{1}_m = \mathbf{1}_n$, we define $\tau(M)$ via the expression

$$\tau(M) = \frac{1}{2} \max_{i,j=1,\ldots,n} ||(e_i - e_j)^\top M||_1. \tag{3}$$

Evidently (3) agrees with both (1) and (2) in the case that $n = m$. Observe that for any triple of indices i, j, l we have $\frac{1}{2}|m_{i,l} - m_{j,l}| = \frac{1}{2}(m_{i,l} + m_{j,l}) - \min\{m_{i,l}, m_{j,l}\}$.

From this it follows that $\tau(M)$ can be rewritten as follows:

$$\tau(M) = \max_{i,j=1,\ldots,n} \left\{ 1 - \sum_{l=1}^{m} \min\{m_{i,l}, m_{j,l}\} \right\}.$$

We note that for the case that M is square, this last expression for $\tau(M)$ appears in [10]. From this extended definition of τ to the rectangular case, we see that if $n \geq 3$ and M happens to have two equal rows, then we may delete one of those rows and maintain the same value of τ.

Let A be an $n \times m$ $(0,1)$ matrix. We say that A has a *scrambling pattern* if, for each pair of indices i, j with $1 \leq i, j \leq n$, $e_i^\top AA^\top e_j \geq 1$. Clearly this is equivalent to the condition that every pair of rows of A has a 1 in a common position. In particular note that if such a matrix A has a scrambling pattern, then it contains at least one 1 in each row. Denote the set of $n \times m$ real matrices by $\mathbb{R}^{n\times m}$. For a $(0,1)$ matrix $A \in \mathbb{R}^{n\times m}$ with a scrambling pattern, we define $\mathcal{S}(A)$ as follows:

$$\mathcal{S}(A) = \{M \in \mathbb{R}^{n\times m} | 0 \leq M \leq A, M\mathbf{1}_n = \mathbf{1}_m\},$$

where the inequalities on M hold entrywise. The main quantity of interest in this paper is then defined as

$$\tau_{\min}(A) = \min\{\tau(M) | M \in \mathcal{S}(A)\}. \tag{4}$$

In particular, note that if D is a directed graph whose $n \times n$ adjacency matrix A has a scrambling pattern, then $\mathcal{S}(A) = \{T | T \text{ is stochastic and } \mathcal{D}(T) \subseteq D\}$ (here we use $\mathcal{D}(T) \subseteq D$ to denote the fact that $\mathcal{D}(T)$ is a spanning subgraph of D). Consequently, we find that $\min\{\tau(T) | T \text{ is stochastic and } \mathcal{D}(T) \subseteq D\} = \tau_{\min}(A)$.

In this paper, we observe that $\tau_{\min}(A)$ can be computed as the solution to a certain linear programming problem. We then go on to establish upper and lower bounds on $\tau_{\min}(A)$ in terms of the number of rows of A, in terms of the row sums of A, and in terms of the column sums of A, characterising the equality cases for each. One of those equality cases turns out to have an intriguing connection with certain balanced incomplete block designs.

Throughout the paper, we make use of basic material from the theory of nonnegative matrices, Markov chains, and combinatorial matrix theory. We refer the reader to [10] for background on the former two topics, and to [2] for background on the latter.

2 Preliminaries

In this section, we collect a few simple results that will be useful in some of our later development. We begin with a little notation and terminology. For an integer $k \in \mathbb{N}$, we will use J_k and I_k to denote the $k \times k$ all ones matrix and identity matrix, respectively, while $\mathbf{1}_k$ and 0_k will denote the all ones vector and zero vector in $\mathbb{R}^k$, respectively. The subscripts will be suppressed when they can be readily determined from the context. Given a vector $x \in \mathbb{R}^n$, we let $diag(x)$ denote the diagonal matrix such that for each $i = 1, \ldots, n$, the i–th diagonal entry is x_i. For an $n \times m$ nonnegative matrix M, and for each $i = 1, \ldots, n$, we denote the *support of row* i, that is, the set of indices l such that $m_{i,l} > 0$, by $supp(i)$, while for each $i, j = 1, \ldots, n$, $S_{i,j}$ will be used to denote $supp(i) \cap supp(j)$. Suppose that M has constant row sums. Then the entries of $(e_i - e_j)^\top M$ sum to 0, and it is straightforward to determine that

$$\frac{1}{2}||(e_i - e_j)^\top M||_1 = \sum_{l=1}^{m} \max\{m_{i,l} - m_{j,l}, 0\} = \sum_{l=1}^{m} \max\{m_{j,l} - m_{i,l}, 0\}.$$

The following lemma will be used in the sequel.

Lemma 2.1. *Let A be a $(0,1)$ matrix, partitioned as $A = \left[\begin{array}{c|c} A_1 & A_2 \end{array}\right]$. If A_1 has at least one 1 in each row, then $\tau_{\min}(A) \le \tau_{\min}(A_1)$.*

Proof. Consider a matrix $M_1 \in \mathcal{S}(A_1)$ such that $\tau(M_1) = \tau_{\min}(A_1)$. Since the matrix $M = \left[\begin{array}{c|c} M_1 & 0 \end{array}\right] \in \mathcal{S}(A)$, we find that $\tau_{\min}(A) \le \tau(M) = \tau(M_1) = \tau_{\min}(A_1)$. □

Our next preliminary result yields a simplification for the case that one column of our matrix dominates another.

Lemma 2.2. *Suppose that A is an $n \times m$ $(0,1)$ matrix of scrambling pattern, written as $A = \left[\begin{array}{c|c} B & x \end{array}\right]$, where B is $n \times (m-1)$. Suppose further that for some $1 \le j \le m-1, Be_j \ge x$. Then $\tau_{\min}(A) = \tau_{\min}(B)$.*

Proof. From Lemma 2.1 we find that $\tau_{\min}(A) \le \tau_{\min}(B)$. Consider a matrix $M \in \mathcal{S}(A)$ such that $\tau(M) = \tau_{\min}(A)$. Without loss of generality, we take $j = 1$, and write M as $M = \left[\begin{array}{c|c|c} u & \overline{M} & v \end{array}\right]$, where u and v are vectors in $\mathbb{R}^n$. Next, we construct the matrix $\left[\begin{array}{c|c|c} u+v & \overline{M} & 0 \end{array}\right] \equiv \left[\begin{array}{c|c} \widehat{M} & 0 \end{array}\right]$. By hypothesis, we have $Be_1 \ge x \ge v$, so that the zero–nonzero pattern of v is contained in that of Be_1. Observing that $\mathbf{1} = M\mathbf{1} = u + v + \overline{M}\mathbf{1} = \widehat{M}\mathbf{1}$, we find further that $0 \le \widehat{M} \le B$. Hence $\widehat{M} \in \mathcal{S}(B)$.

For each pair of indices p and q with $1 \le p, q \le m$, we have

$$|(u_p + v_p) - (u_q + v_q)| \le |u_p - u_q| + |v_p - v_q|,$$

from which it follows that $\tau(\left[\begin{array}{c|c} \widehat{M} & 0 \end{array}\right]) = \tau(\widehat{M}) \le \tau(M)$. Consequently, we find that $\tau_{\min}(B) \le \tau\left(\left[\begin{array}{c|c} \widehat{M} & 0 \end{array}\right]\right) \le \tau(M) = \tau_{\min}(A)$. The conclusion now follows. □

We now provide a parallel result for the case that one row dominates another.

Lemma 2.3. *Suppose that A is an $n \times m$ $(0,1)$ matrix with a scrambling pattern. Suppose that for some $2 \le j \le n, e_1^\top A \ge e_j^\top A$. Then $\tau_{\min}(A) = \tau_{\min}(B)$, where B is the matrix constructed from A by deleting its first row.*

Proof. Without loss of generality, we assume that $e_1^\top A \geq e_2^\top A$. First, select $\overline{M} \in \mathcal{S}(B)$ such that $\tau(\overline{M}) = \tau_{\min}(B)$. Letting

$$\widehat{M} = \left[\begin{array}{c} e_1^\top \overline{M} \\ \hline \overline{M} \end{array} \right],$$

it follows readily that $\widehat{M} \in \mathcal{S}(A)$, and that $\tau(\widehat{M}) = \tau(\overline{M})$. Hence $\tau_{\min}(A) \leq \tau_{\min}(B)$. Next, select $M \in \mathcal{S}(A)$ such that $\tau(M) = \tau_{\min}(A)$, and let M_0 be the matrix constructed from M by deleting its first row. Evidently $\tau(M) \geq \tau(M_0)$, and we now find readily that $\tau_{\min}(A) = \tau(M) \geq \tau(M_0) \geq \tau_{\min}(B)$. □

In view of Lemmas 2.2 and 2.3, we see that in order to find $\tau_{\min}(A)$ for a $(0, 1)$ matrix A, there is no loss of generality in assuming that no column of A dominates another entrywise, and that no row of A dominates another entrywise. We will have occasion to make that assumption in the sections that follow.

3 Bounds on $\tau_{\min}$

Suppose that A is an $n \times m$ $(0, 1)$ matrix with a scrambling pattern, and note that the task of computing $\tau_{\min}(A)$ is equivalent to that of solving the following optimisation problem:

$$\begin{aligned} &\text{minimise}: \ \frac{1}{2}\max\{||e_i^\top T - e_j^\top T||_1 | 1 \leq i < j \leq n\} \\ &\text{subject to}: \ T \in \mathcal{S}(A). \end{aligned} \tag{5}$$

Using standard techniques outlined in [1, section 1.2.2], the problem (5) can be converted into a linear programming problem in standard form; the linear programme has $\mathbf{1}^\top A \mathbf{1} + 1$ variables and $\mathbf{1}^\top A \mathbf{1} + n + \sum_{1 \leq i < j \leq n} 2^{|S_{i,j}|}$ constraint equalities and inequalities. Thus, in principal, when A is given, $\tau_{\min}(A)$ can be computed by using standard linear programming techniques. However, as noted in [1, section 1.2.2], for a linear programming problem having p variables and q constraints, the complexity of computing a solution (via interior point methods) is of order $p^2 q$. In particular, if some $|S_{i,j}|$ is sufficiently large, the number of constraints may be exponential in m. The possibility that the computational complexity of finding $\tau_{\min}(A)$ is exponential in m motivates us to investigate other avenues for gaining insight into $\tau_{\min}$. For this reason, in this section we focus on finding readily computable upper and lower bounds on $\tau_{\min}$.

While we will not pursue the linear programming viewpoint on $\tau_{\min}$ any further in this paper, that viewpoint does yield one interesting fact. A standard result (see [1, section 4.2]) asserts that the family of solutions to a feasible linear programming problem forms a convex set. Consequently, the following is immediate.

Proposition 3.1. *Suppose that A is an $n \times m$ $(0,1)$ matrix with a scrambling pattern. Then the set*

$$\{M \in \mathcal{S}(A) | \tau(M) = \tau_{\min}(A)\}$$

is convex.

3.1 Bounds via the number of rows

Suppose that $k \in \mathbb{N}$ with $k \geq 2$. We recursively define the following $k \times \binom{k}{2}$ matrix $A(k)$ as follows: $A(2) = \mathbf{1}_2$,

$$A(k+1) = \left[\begin{array}{c|c} \mathbf{1}_k^\top & 0^\top_{\binom{k}{2}} \\ \hline I_k & A(k) \end{array} \right], k \in \mathbb{N}.$$

So, for example when $k = 5$ we have

$$A(5) = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \end{bmatrix}.$$

Observe that each column of $A(k)$ contains exactly two 1s, and that each pair of distinct rows of $A(k)$ have supports that intersect in exactly one element. Label the columns of $A(k)$ in lexicographic order as $(1,2),(1,3),\ldots,(1,k),(2,3),(2,4),\ldots,$ $(2,k),\ldots,(k-1,k)$, and observe that for any i,j with $1 \leq i < j \leq k, e_i^\top A(k)$ and $e_j^\top A(k)$ have a single 1 in a common position, namely the position corresponding to column indexed by the ordered pair (i,j).

Our initial goal in this subsection is to establish an attainable upper bound on $\tau_{\min}(A)$ in terms of the number of rows in A. We do so via a sequence of helpful results. We begin our discussion with a claim that for an $n \times m$ $(0,1)$ matrix A with a scrambling pattern, there is no loss of generality in assuming that each column of A contains at least two 1s. To see the claim, suppose that Ae_j has at most one 1. If it happens that $Ae_j = 0$, then by Lemma 2.2,we have $\tau_{\min}(A) = \tau_{\min}(\tilde{A})$ where $\tilde{A}$ is formed from A by deleting its j–th column. On the other hand, if Ae_j has just one 1, with $Ae_j = e_i$, say, then either there is an $l \neq j$ such that $a_{i,l} = 1$, or we have $e_i^\top A = e_j^\top$. In the former case, we have $Ae_l \geq Ae_j$, and again by Lemma 2.2 we may delete the j–th column from A without changing the value of $\tau_{\min}$. In the latter case, since A has a scrambling pattern, and since the only nonzero entry of row i is in column j, it must be the case that some (in fact every) row of A dominates its i–th row. But then Ae_j has at least two 1s, contrary to our hypothesis. This establishes the claim.

Lemma 3.1. *Suppose that A is an $n \times m$ $(0,1)$ matrix with a scrambling pattern. Then $\tau_{\min}(A) \leq \frac{n-2}{n-1}$.*

Proof. From Lemma 2.2 and 2.3, we may assume without loss of generality that no row of A dominates another, and that no column of A dominates another; from the claim preceding this lemma, we may assume that each column of A contains at least two 1s.

For each pair of indices i,j with $1 \le i < j \le m$, let $\mathsf{e}_{(i,j)}$ be the vector in $\mathbb{R}^{\binom{n}{2}}$ having a 1 in the position corresponding to (i,j), and 0s elsewhere. For $1 \le i < j \le m$, we then define the set $\Sigma(i,j) = \{l | Ae_l \ge A(n)\mathsf{e}_{(i,j)}\}$; observe that this set is not empty. Now let B be the $\binom{n}{2} \times m$ $(0,1)$ matrix such that for each $1 \le i < j \le n, 1 \le l \le m$, the entry of B in row (i,j) and column l is 1 if $l \in \Sigma(i,j)$ and 0 otherwise. Note that each row of B contains at least one 1, and so the diagonal matrix $D = diag(B\mathbf{1})$ is nonsingular. Next, we consider the $n \times m$ matrix $M = \frac{1}{n-1}A(n)D^{-1}B$. Evidently M is nonnegative and $M\mathbf{1} = \frac{1}{n-1}A(n)\mathbf{1} = \mathbf{1}$. Note that for each $1 \le l \le m$, Me_l is a linear combination of the columns of the form $A(n)\mathsf{e}_{(i,j)}$ where the pairs (i,j) all have the property that $l \in \Sigma(i,j)$. In particular, $Me_l \le Ae_l$ for each such l, and we thus deduce that $M \in \mathcal{S}(A)$.

Now $\tau(M) \le \tau(\frac{1}{n-1}A(n))\tau(D^{-1}B) \le \tau(\frac{1}{n-1}A(n))$. Further, we observe that each nonzero entry of $\frac{1}{n-1}A(n)$ is $\frac{1}{n-1}$, and that for each $1 \le i < j \le n$, $\frac{1}{n-1}e_i^\top A(n)\mathsf{e}_{(i,j)} = \frac{1}{n-1}e_j^\top A(n)\mathsf{e}_{(i,j)} = \frac{1}{n-1}$. We thus find that $\tau(\frac{1}{n-1}A(n)) = \frac{n-2}{n-1}$, from which the conclusion follows. $\square$

The following result will turn out to be quite useful. We will revisit some of its consequences in subsections 3.3 and 3.4

Proposition 3.2. *Suppose that A is a $n \times m$ $(0,1)$ matrix with scrambling pattern. Fix an index i between 1 and n, and let B be the submatrix of A on rows $1,\ldots,n$ and columns indexed by $supp(i)$. Suppose that there is a collection of l rows of B such that in the corresponding $l \times |supp(i)|$ submatrix of B, each column contains at least c 0s. Then $\tau_{\min}(A) \ge \frac{c}{l}$.*

Proof. Without loss of generality we suppose that $i = 1, supp(i) = \{1,\ldots,p\}$, and that the l rows in the hypothesis are rows $2,\ldots,l+1$. Suppose that $M \in \mathcal{S}(A)$. Fix an index i with $2 \le i \le l+1$. Since the entries of $(e_1 - e_l)^\top M$ sum to zero, it follows that $\frac{1}{2}||(e_1 - e_l)^\top M||_1$ coincides with the sum of the positive entries of the vector $(e_1 - e_l)^\top M$. It now follows that for each $i = 2,\ldots,l+1$,

$$\frac{1}{2}||(e_1 - e_i)^\top M||_1 \ge \sum_{j=1,\ldots,p,a_{i,j}=0} m_{1,j}.$$

Consequently, we have

$$\begin{aligned} l\tau(M) &\ge \sum_{i=2}^{l+1} \frac{1}{2}||(e_1 - e_i)^\top M||_1 \ge \sum_{i=2}^{l+1} \sum_{j=1,\ldots,p,a_{i,j}=0} m_{1,j} \\ &= \sum_{j=1}^{p} \sum_{i=2,\ldots,l+1,a_{i,j}=0} m_{1,j} \ge c\sum_{j=1}^{p} m_{1,j} = c. \end{aligned}$$

The conclusion now follows. $\square$

Proposition 3.2 is used to establish the following result.

Corollary 3.1. *Suppose that A is an $n \times m$ $(0,1)$ matrix with a scrambling pattern. Fix an index i between 1 and n, and suppose that for each $l \in supp(i)$, Ae_l contains at most two 1s. Then $\tau_{\min}(A) = \frac{n-2}{n-1}$.*

Proof. Evidently there is a $(n-1) \times |supp(i)|$ submatrix of A having at least $n-2$ 0s in each column that satisfies the hypotheses of Proposition 3.2. Hence $\tau_{\min}(A) \geq \frac{n-2}{n-1}$, and since $\tau_{\min}(A) \leq \frac{n-2}{n-1}$ by Lemma 3.1, the conclusion follows. $\square$

The following technical result will assist in the proof of Theorem 3.1 below.

Lemma 3.2. *Let A be an $n \times m$ $(0,1)$ matrix with scrambling pattern and suppose that for each $i = 1, \ldots, n$, there is an $l \in supp(i)$ such that Ae_l contains at least three 1s. Then $\tau_{\min}(A) \leq \frac{n-3}{n-2}$.*

Proof. Consider $i = 1$, and without loss of generality, we take $supp(1) = \{1, \ldots, q\}$. By permuting rows $2, \ldots, n$ and columns $1, \ldots, q$ if necessary, we find that for some $1 \leq p \leq q$, the submatrix of A on its first q columns has the form

$$\left[\begin{array}{ccccc|c} \multicolumn{5}{c|}{\mathbf{1}_p^\top} & \mathbf{1}_{q-p}^\top \\ \hline \mathbf{1}_{r_1} & * & \ldots & * & * & * \\ 0_{r_2} & \mathbf{1}_{r_2} & \ldots & * & * & * \\ \vdots & & \ddots & & \vdots & \vdots \\ 0_{r_p} & 0_{r_p} & \ldots & 0_{r_p} & \mathbf{1}_{r_p} & * \end{array}\right],$$

where $r_1 \geq 2$ and $r_j \geq 1, j = 2, \ldots, p$. (Here the $*$ entries correspond to positions for which the entries in A do not need to be specified for the purposes of the proof.) Next we note that it suffices to consider the case that $p = q$, for if $p < q$, we may zero out the entries in the first row of A in positions $p+1, \ldots, q$ to generate a matrix $\tilde{A}$ such that $\tau_{\min}(A) \leq \tau_{\min}(\tilde{A})$. As this zeroing out process only affects entries in the first row of A, we deduce that $\tilde{A}$ also has a scrambling pattern.

So, taking p equal to q, we find that $n - 1 = \sum_{j=1}^{q} r_j \geq 2 + (q-1)$, so that $q \leq n-2$. A similar argument applies to the cases $i = 2, \ldots, n$, and it follows that A dominates a $(0,1)$ matrix B such that
i) B has a scrambling pattern and
ii) $e_i^\top B\mathbf{1} \leq n-2, i = 1, \ldots, n$.
Since $B \leq A$, we have $\mathcal{S}(B) \subseteq \mathcal{S}(A)$, and hence $\tau_{\min}(A) \leq \tau_{\min}(B)$.

Let $D = diag(B\mathbf{1})$, and consider $M = D^{-1}B$. Note that $M \in \mathcal{S}(B)$ and that each nonzero entry of M is bounded below by $\frac{1}{n-2}$. Select indices $1 \leq i < j \leq n$, and note that

$$\frac{1}{2}||(e_i - e_j)^\top M||_1 = 1 - \sum_{l \in S_{i,j}} \min\{m_{i,l}, m_{j,l}\} \leq 1 - \frac{1}{n-2}.$$

Hence we have $\frac{n-3}{n-2} \geq \tau_{\min}(B) \geq \tau_{\min}(A)$, as desired.

$\square$

Here is one of the main results in this subsection. It follows directly from Lemma 3.1, Corollary 3.1 and Lemma 3.2.

Theorem 3.1. *Let A be an $n \times m$ $(0,1)$ matrix with scrambling pattern. Then*

$$\tau_{\min}(A) \leq \frac{n-2}{n-1}. \tag{6}$$

Equality holds in (6) if and only if there is an index $i = 1, \ldots, n$, such that for each $l \in supp(i)$, Ae_l contains at most two 1s.

We now provide a lower bound to complement Theorem 3.1.

Theorem 3.2. *Let A be an $n \times m$ $(0,1)$ matrix with scrambling pattern. If A does not contain an all–ones column, then*

$$\tau_{\min}(A) \geq \frac{1}{n-1}. \tag{7}$$

Equality holds in (7) if and only if A contains a $n \times n$ submatrix that, up to row and column permutations, has the form $J_n - I_n$.

Proof. Let B be the submatrix of A on the columns in $supp(1)$. Since each column of A (and hence B) contains at least one 0, it follows from Proposition 3.2 that $\tau_{\min}(A) \geq \frac{1}{n-1}$.

Suppose now that equality holds in (7). Again referring to Proposition 3.2, we find that if $\widehat{B}$ is an $l \times |supp(1)|$ submatrix of B having a 0 in each column, then necessarily $l = n-1$ (and $\widehat{B} = B$). Evidently a similar observation applies to the submatrix of A on the columns in $supp(i)$, for each $i = 1, \ldots, n$. Next, we examine the structure of A, and we note that it suffices to consider the case that no row of A dominates another, and no column of A dominates another. Permuting the columns of A if necessary, it follows that the first row of A can be written as $\left[\begin{array}{cc} 0_{l_1}^\top & \mathbf{1}_{m-l_1}^\top \end{array}\right]$, for some $1 \leq l_1 \leq m-1$. Since column l_1+1 contains a zero outside of the first row, it follows that (again, permuting rows and columns if necessary) the first two rows of A can be written as

$$\left[\begin{array}{ccc} 0_{l_1}^\top & \mathbf{1}_{l_2}^\top & \mathbf{1}_{m-l_1-l_2}^\top \\ * & 0_{l_2}^\top & \mathbf{1}_{m-l_1-l_2}^\top \end{array}\right],$$

for some $1 \leq l_2 \leq m-l_1-1$. (Here the star represents entries yet to be determined.) Continuing in this way, we find that for each $i \leq n-1$, $e_i^\top A$ has the form

$$\left[\begin{array}{ccc} * & 0_{l_i}^\top & \mathbf{1}_{m-l_1-\ldots-l_{i-1}}^\top \end{array}\right],$$

for some $1 \le l_2 \le m - l_1 - \ldots - l_{i-1} - 1$. Similarly, we find that $e_n^\top A = \begin{bmatrix} * & 0_{l_n}^\top \end{bmatrix}$. Consequently, we see that A has the form

$$\begin{bmatrix} 0 & \ldots & 0 & 1 & \ldots & 1 & & \ldots & & 1 & \ldots & 1 \\ * & \ldots & * & 0 & \ldots & 0 & 1 & \ldots & 1 \ \ldots & 1 & \ldots & 1 \\ \vdots & & & & & \ddots & & & & \vdots & & \\ * & \ldots & * & * & \ldots & * & 0 & \ldots & 0 & 1 & \ldots & 1 \\ * & \ldots & * & * & \ldots & * & * & \ldots & * & 0 & \ldots & 0 \end{bmatrix}. \tag{8}$$

Next, we note that all of the star entries on the bottom row must be 1s, otherwise the last column of A dominates some other column. Now considering the second last row of A, we see again that all of the star entries must be 1s, otherwise one column of A dominates another. Continuing, we find that all of the star entries in (8) must be 1s. We now find readily that some submatrix of A can be permuted to the form $J_n - I_n$.

Finally, if A contains $J_n - I_n$ as a submatrix, we find from Lemma 2.1 that $\tau_{\min}(A) \le \tau_{\min}(J_n - I_n) = \frac{1}{n-1}$, so that equality holds in (7). $\square$

Suppose that T is a $n \times n$ stochastic matrix with zero diagonal, and label the eigenvalues of T as $1 \equiv \lambda_1, \lambda_2, \ldots, \lambda_n$. In [6] it is shown that $\max_{j=2,\ldots,n} |\lambda_j| \ge \frac{1}{n-1}$. Since $\tau(T) \ge \max_{j=2,\ldots,n} |\lambda_j|$, we see that for any such T, $\tau(T) \ge \frac{1}{n-1}$. This provides an alternate proof of (7) in the special case that A is $n \times n$ and has zero diagonal.

3.2 A bound via the maximum row sum

Here is a bound on $\tau_{\min}(A)$ based on the row sums of A.

Proposition 3.3. *Let A be an $n \times m$ $(0,1)$ matrix with a scrambling pattern, and let $p = A\mathbf{1}$. Then*

$$\tau_{\min}(A) \le \max_{1 \le i < j \le n} \Big\{ 1 - \frac{|S_{i,j}|}{\max\{p_i, p_j\}} \Big\}. \tag{9}$$

Proof. Let $D = diag(p)$, and observe that the matrix $M = D^{-1}A \in \mathcal{S}(A)$. Since $\tau_{\min}(A) \le \tau(M)$, (9) follows immediately. $\square$

We have the following consequence of Proposition 3.3.

Corollary 3.2. *Suppose that D is a directed graph on vertices $1, \ldots, n$. For each $i = 1, \ldots, n$, denote the outdegree of vertex i by p_i, and for each $1 \le i < j \le n$, let $\sigma(i,j)$ denote the number of vertices k such that $i \to k$ and $j \to k$ in D. Then there is a stochastic matrix T of order n having eigenvalues $1, \lambda_2, \ldots, \lambda_n$ such that:*
i) $\mathcal{D}(T)$ is a spanning subgraph of D; and
ii) $\max\{|\lambda_2|, \ldots, |\lambda_n|\} \le \max_{1 \le i < j \le n} \Big\{ 1 - \frac{|\sigma(i,j)|}{\max\{p_i, p_j\}} \Big\}$.

Proof. Denote the adjacency matrix of D by A, and select a matrix $T \in \mathcal{S}(A)$ such that $\tau(T) = \tau_{\min}(A)$. Since $T \in \mathcal{S}(A)$, i) holds. Let the non–Perron eigenvalues of T be $\lambda_2, \ldots, \lambda_n$, and recall that, as noted in section 1, $\tau(T)$ is an upper bound on the modulus of any non–Perron eigenvalue of T. Hence we find that $\max\{|\lambda_2|, \ldots, |\lambda_n|\} \leq \tau(T) = \tau_{\min}(A)$, while from Proposition 3.3 we find that $\tau_{\min}(A) \leq \max_{1\leq i<j\leq n} \left\{1 - \frac{|\sigma(i,j)|}{\max\{p_i, p_j\}}\right\}$. Conclusion ii) now follows. □

Next we present the main result of this subsection.

Theorem 3.3. *Let A be an $n \times m$ $(0,1)$ matrix with a scrambling pattern, let $p = A\mathbf{1}$, and set $\overline{p} = \max\{p_i | i = 1, \ldots, n\}$. Then*

$$\tau_{\min}(A) \leq 1 - \frac{1}{\overline{p}}. \tag{10}$$

Equality holds in (10) *if and only if there is an index i between* 1 *and n such that:*
i) $p_i = \overline{p}$, and
ii) for each $l \in supp(i)$, there is an index j between 1 *and n such that $S_{i,j} = \{l\}$.*

Proof. The upper bound (10) follows immediately from Proposition 3.3.

To address the case of equality in (10), suppose first that there is an index i satisfying conditions i) and ii). Without loss of generality we take $i = 1$ and $supp(i) = \{1, \ldots, \overline{p}\}$. Let B be the submatrix of A on columns $1, \ldots, \overline{p}$. From i) and ii), it follows that for each l between 1 and $\overline{p}$, there is an index j such that $e_j^\top B = e_j^\top$. Hence, there is a collection of $\overline{p}$ rows of B such that the corresponding submatrix of B is (up to row and column permutations) $I_{\overline{p}}$. From Proposition 3.2 we find that $\tau_{\min}(A) \geq \frac{\overline{p}-1}{\overline{p}}$, and thus it must be the case that $\tau_{\min}(A) = \frac{\overline{p}-1}{\overline{p}}$.

For the converse implication, suppose now that for each i between 1 and n, either condition i) or condition ii) fails to hold. Then in particular, for each i such that $p_i = \overline{p}$, there is an index $l \in supp(i)$ such that for every j between 1 and n, either $l \notin S_{i,j}$ or $|S_{i,j}| \geq 2$. Fixing such an index i, we see that there is an index $l \in supp(i)$ such that for each j with $1 \leq j \leq n$ and $j \neq i$, either $a_{j,l} = 0$, or there is an index $l_j \neq l$ such that $a_{i,l_j} = a_{j,l_j} = 1$. Consequently, the matrix $\widehat{A} = A - e_i e_l^\top$ is a $(0,1)$ matrix with a scrambling pattern; clearly $\tau_{\min}(A) \leq \tau_{\min}(\widehat{A})$, and the i–th row sum of $\widehat{A}$ is $\overline{p} - 1$. Iterating the procedure if necessary, it follows that we may successively zero out 1s from A in order to produce a matrix $\tilde{A}$ with a scrambling pattern whose maximum row sum is at most $\overline{p} - 1$. But then we have $\tau_{\min}(A) \leq \tau_{\min}(\tilde{A}) \leq 1 - \frac{1}{\overline{p}-1}$, so that strict inequality holds in (10).

□

Our results above enable us to address the problem of finding $\tau_{\min}(A)$ for any $(0,1)$ matrix A with four rows.

Example 3.1. In this example we identify the values of $\tau_{\min}$ for matrices of scrambling pattern having just four rows. Suppose that A is a $4 \times m$ $(0,1)$ matrix of scrambling pattern, and that $m \geq 2$. We assume that no column of A is equal to $\mathbf{1}_4$, otherwise $\tau_{\min}(A) = 0$. Without loss of generality, we assume henceforth that no row of A dominates another, and that no column of A dominates another.

From the assumption that no column of A dominates another, and that no column of A is $\mathbf{1}_4$, we find that each column of A contains either two or three 1s. Hence each column of A is a member of either the set

$$V_1 = \left\{ \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \right\}$$

or the set

$$V_2 = \left\{ \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \end{bmatrix} \right\}.$$

If A contains no columns from V_2, then, up to row and column permutations, necessarily A is given by

$$A_1 = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}.$$

Observing that this A satisfies conditions i) and ii) of Theorem 3.3, we see that $\tau_{\min}(A_1) = \frac{2}{3}$.

If A contains just one column from V_2, we find that, up to row and column permutations, A is given by

$$A_2 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}.$$

Again appealing to Theorem 3.3 we see that $\tau_{\min}(A_2) = \frac{2}{3}$.

If A contains two or three columns from V_2, we find the up to row and column permutations, A is given by either

$$A_3 = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}$$

or

$$A_4 = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix},$$

respectively. From Theorem 3.3 it follows that $\tau_{\min}(A_3) = \frac{1}{2}$ and $\tau_{\min}(A_4) = \frac{1}{2}$.

Finally, if A has four columns from V_2, then it contains $J_4 - I_4$ as a submatrix, and appealing to Theorem 3.2 again, we have $\tau_{\min}(A) = \frac{1}{3}$.

3.3 A bound via the maximum column sum

This subsection contains an application of Proposition 3.2 that leads to a lower bound on $\tau_{\min}$ whose equality case has an interesting characterisation.

Theorem 3.4. *Let A be an $n \times m$ $(0,1)$ matrix of scrambling pattern, and suppose that each column of A contains at least c 0s. Then*

$$\tau_{\min}(A) \geq \frac{c}{n-1}. \tag{11}$$

Equality holds in (11) if and only if there is a diagonal matrix D of order m with nonnegative diagonal entries such that $ADA^\top = \frac{c}{n-1}I + (1 - \frac{c}{n-1})J$. In particular, if equality holds in (11), then A has exactly c 0s in each column that corresponds to a positive diagonal entry in D.

Proof. The lower bound on (11) follows immediately from Proposition 3.2.

In order to establish the characterisation of equality, suppose first that equality holds in (11), and let M be a matrix in $\mathcal{S}(A)$ such that $\tau(M) = \frac{c}{n-1}$. Suppose without loss of generality that $\frac{1}{2}||(e_1 - e_2)^\top M||_1 = \frac{c}{n-1}$. We then have

$$\frac{c}{n-1} \geq \frac{1}{n-1}\sum_{i=2}^{n}\frac{1}{2}||(e_1 - e_i)^\top M||_1 \geq \frac{1}{n-1}\sum_{i=2}^{n}\sum_{l \ni m_{i,l}=0} m_{1,l},$$

where the second inequality follows from the fact that for each $2 \leq i \leq n$, $\frac{1}{2}||(e_1 - e_i)^\top M||_1$ is equal to the sum of the nonnegative entries in the vector $(e_1 - e_i)^\top M$. Further, from the hypothesis, for each $1 \leq l \leq m$, there are at least c indices i such that $m_{i,l} = 0$, and consequently, we find that $\sum_{i=2}^{n}\sum_{l \ni m_{i,l}=0} m_{1,l} \geq c\sum_{l \in supp(1)} m_{1,l}$. Assembling these observations, we have

$$\begin{aligned}\frac{c}{n-1} \geq \frac{1}{n-1}\sum_{i=2}^{n}\frac{1}{2}||(e_1 - e_i)^\top M||_1 \geq \frac{1}{n-1}\sum_{i=2}^{n}\sum_{l \ni m_{i,l}=0} m_{1,l} \geq \frac{c}{n-1}\sum_{l \in supp(1)} m_{1,l} \\ = \frac{c}{n-1}.\end{aligned}$$

We thus deduce that for each $i = 2, \ldots, n$, $\frac{1}{2}||(e_1 - e_i)^\top M||_1 = \frac{c}{n-1}$, and it now follows that for any pair of indices p, q with $1 \leq p < q \leq n$, we have $\frac{1}{2}||(e_p - e_q)^\top M||_1 = \frac{c}{n-1}$. Indeed, it must also be the case that for each such p and q,

$$\frac{1}{2}||(e_p - e_q)^\top M||_1 = \sum_{l \ni m_{q,l}=0} m_{p,l}. \tag{12}$$

From (12) and the fact that for each $p \neq q$, $\frac{1}{2}||(e_p - e_q)^\top M||_1$ is equal to the sum of the nonnegative entries in the vector $(e_1 - e_i)^\top M$, we see that for each pair of distinct indices p, q,

$$\sum_{l \ni m_{q,l}=0} m_{p,l} = \sum_{l \ni m_{p,l} \geq m_{q,l}} (m_{p,l} - m_{q,l}) = \sum_{l \ni m_{q,l}=0} m_{p,l} + \sum_{l \ni m_{p,l} \geq m_{q,l} > 0} (m_{p,l} - m_{q,l}),$$

and hence

$$\sum_{l \ni m_{p,l} \geq m_{q,l} > 0} (m_{p,l} - m_{q,l}) = 0. \tag{13}$$

Next we claim that in each column of M, all of the positive entries are equal. To see the claim, suppose to the contrary that for some triple of indices p, q, l, we have $m_{p,l} > m_{q,l} > 0$. But then we have $m_{p,l} \geq m_{q,l} > 0$ and $(m_{p,l} - m_{q,l}) > 0$, which contradicts (13). Consequently, in each column of M, all of the positive entries are equal, as claimed.

Hence M can be written as AD for some diagonal matrix D with nonnegative entries. Further, since $\frac{1}{2}||(e_p - e_q)^\top M||_1 = 1 - \sum_{l=1}^m \min\{m_{p,l}, m_{q,l}\} = 1 - e_p^\top M A^\top e_q$, it follows that $e_p^\top M A^\top e_q = 1 - \frac{c}{n-1}$ whenever $p \neq q$. Observing that $e_p^\top M A^\top e_p = \sum_{l=1}^m m_{p,l} = 1$ for each $p = 1, \ldots, n$, we thus find that $MA^\top = ADA^\top = \frac{c}{n-1} I + (1 - \frac{c}{n-1})J$. Finally, we note that since $\mathbf{1}^\top ADA^\top = (n-c)\mathbf{1}^\top$, and since $\mathbf{1}^\top A \leq (n-c)\mathbf{1}^\top$ by hypothesis, we have that

$$(n-c)\mathbf{1}^\top = \mathbf{1}^\top ADA^\top \leq (n-c)\mathbf{1}^\top DA^\top = (n-c)(AD\mathbf{1})^\top = (n-c)\mathbf{1}^\top.$$

It now follows that necessarily we must have $\mathbf{1}^\top A e_l = (n-c)e_l$ whenever $d_l > 0$.

Conversely, if there is a nonnegative and diagonal matrix D such that $ADA^\top = \frac{c}{n-1} I + (1 - \frac{c}{n-1})J$, we find readily that the matrix AD is in $\mathcal{S}(A)$. Further, for each pair of distinct indices p and q, we find that $\frac{1}{2}||(e_p - e_q)^\top AD||_1 = 1 - e_p^\top ADA^\top e_q = \frac{c}{n-1}$. Hence $\tau_{\min}(A) \leq \tau(AD) = \frac{c}{n-1}$, so that equality holds in (11). $\square$

3.4 Mock designs

Suppose that A is an $n \times m$ $(0,1)$ matrix with at least $c \geq 1$ 0s in each column. If there is a diagonal matrix D having nonnegative diagonal entries such that $ADA^\top = \frac{c}{n-1} I + (1 - \frac{c}{n-1})J$, then we say that the pair (A, D) is a *mock design*. The motivation for this term is as follows. Suppose that A is the incidence matrix of a balanced incomplete block design with parameters (v, k, λ), where $v = n, k = n - c$ and $\lambda = \frac{m(n-c)(n-c-1)}{n(n-1)}$ (we refer the reader to [9, section 6.2] for background on block designs). Set $r = \frac{\lambda(n-1)}{n-1-c} = \frac{m(n-c)}{n}$. Then $AA^\top = (r - \lambda)I + \lambda J$, so that taking $D = \frac{1}{r} I_m$, we find that $ADA^\top = \frac{c}{n-1} I + (1 - \frac{c}{n-1})J$. Thus, any balanced incomplete block design gives rise to a mock design. In this section we explore some of the properties of mock designs.

Given a $p \times q$ $(0,1)$ matrix A, we let $comp(A)$ be the $\binom{p}{2} \times q$ matrix whose rows are given by $e_i^\top A \circ e_j^\top A$, written in lexicographic order, where $\circ$ denotes the Hadamard product. Our next result yields some insight into the relationship between A and D when the pair (A, D) is a mock design.

Proposition 3.4. *Let A be an $n \times m$ $(0,1)$ matrix with $c \geq 1$ 0s in each column. Suppose that for some nonnegative diagonal matrix D_0, the pair (A, D_0) is a mock design, and let $\Delta = \{D | (A, D)$ is a mock design$\}$. Then Δ is a convex set. Further, D is an extreme point of Δ if and only if:*
i)

$$\left[\frac{A}{comp(A)}\right](D\mathbf{1}) = \left[\frac{\mathbf{1}_n}{(1-\frac{c}{n-1})\mathbf{1}_{\binom{n}{2}}}\right]; \text{ and}$$

ii) letting $P = \{j | d_j > 0\}$, the submatrix of

$$\left[\frac{A}{comp(A)}\right]$$

on the columns indexed by P is of full column rank.

Proof. Observing that we can write Δ as

$$\Delta = \left\{ diag(x) \middle| x \geq 0, \left[\frac{A}{comp(A)}\right] x = \left[\frac{\mathbf{1}_n}{(1-\frac{c}{n-1})\mathbf{1}_{\binom{n}{2}}}\right] \right\},$$

it is now straightforward to determine that Δ is a convex set.

Let $x \geq 0$ be a vector such that $diag(x) \in \Delta$, and let $P = \{j | x_j > 0\}$. If $diag(x)$ is an extreme point of Δ, then certainly the submatrix of

$$\left[\frac{A}{comp(A)}\right]$$

on the columns indexed by P has nullity zero, otherwise we can find a nonzero null vector y of

$$\left[\frac{A}{comp(A)}\right]$$

such that $diag(x+y), diag(x-y) \in \Delta$. But then in that case, $diag(x) = \frac{1}{2}diag(x+y) + \frac{1}{2}diag(x-y)$, contrary to our assumption that $diag(x)$ is an extreme point of Δ.

Conversely, suppose that the submatrix S of

$$\left[\frac{A}{comp(A)}\right]$$

on the columns indexed by P has full column rank, and suppose that x is a vector such that $diag(x) \in \Delta$. Write x as $x = \sum_{j=1}^{r} \alpha_j y(j)$, where $\alpha_j > 0, j = 1, \ldots, r, \sum_{j=1}^{r} \alpha_j = 1$, and $diag(y(j)) \in \Delta$, for $j = 1, \ldots, r$. Note that necessarily, each vector $y(j)$ has support contained in P. Fix an index j, and let z be the subvector of $y(j)$ on the rows indexed by P. We have $Sz = \left[\begin{array}{c} \mathbf{1}_n \\ \hline (1-\frac{c}{n-1})\mathbf{1}_{\binom{n}{2}} \end{array}\right]$, and since S has full column rank, it must be the case that $z_i = x_i$ for each $i \in P$. It now follows that $y(j) = x$ for each $j = 1, \ldots, r$, so that x is an extreme point of Δ. $\square$

Example 3.2. Here is an example of an 8×24 $(0,1)$ matrix A with three 0s in each column:

$$A = \begin{bmatrix} 0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1 \\ 0&0&1&1&1&1&0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1 \\ 1&1&0&0&1&1&0&0&0&1&1&1&1&0&0&0&0&0&1&1&1&1&1&1 \\ 1&1&1&1&0&1&0&1&1&0&0&1&1&0&0&1&1&1&1&1&1&0&0&0 \\ 1&1&1&1&0&1&1&0&1&1&1&0&1&1&1&0&1&1&0&0&0&1&1&1 \\ 1&1&0&1&1&0&1&1&1&0&1&1&0&1&1&0&0&1&1&0&0&1&0&0 \\ 0&1&1&0&1&1&1&1&1&1&0&1&0&0&1&1&1&0&0&1&0&0&1&0 \\ 1&0&1&1&1&0&1&1&0&1&1&0&1&1&0&1&0&0&0&0&1&0&0&1 \end{bmatrix}.$$

Letting d be the vector given by

$$d = \frac{1}{35}\left[\begin{array}{cccccccccccccccccccccccc} 3&3&3&3&6&3&1&4&1&4&1&2&2&2&3&2&1&1&3&1&3&2&1&1 \end{array}\right]^\top,$$

a computation shows that $Adiag(d)A^\top = \frac{3}{7}I + \frac{4}{7}J$; hence $(A, diag(d))$ is a mock design. Further, it can be verified that the matrix

$$\left[\begin{array}{c} A \\ \hline comp(A) \end{array}\right]$$

has full column rank. Thus it follows from Proposition 3.4 that the set $\Delta = \{D|(A,D) \text{ is a mock design}\}$ consists of a single element, namely $diag(d)$.

Example 3.3. We consider the 6×18 matrix A given by

$$A = \begin{bmatrix} 1&1&1&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&1&1&1&1&1&1&1&1&1&0&0&0&0 \\ 0&0&1&1&0&0&0&1&1&1&1&0&0&0&1&1&1&0 \\ 1&1&0&0&0&0&1&0&1&0&0&1&1&0&1&1&0&1 \\ 0&1&0&1&0&1&0&0&0&1&0&1&0&1&1&0&1&1 \\ 1&0&1&0&1&0&0&0&0&0&1&0&1&1&0&1&1&1 \end{bmatrix},$$

and observe that A has three 0s in each column. Our goal here is to find the extreme points of the polytope $\Delta = \{D|D \text{ is diagonal and } (A,D) \text{ is a mock design}\}$. In order to do so, we first consider the vectors $c_1, \ldots, c_4$ given respectively as follows:

$$\frac{1}{5}\left[\begin{array}{cccccccccccccccccc} 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{array}\right]^\top,$$
$$\frac{1}{5}\left[\begin{array}{cccccccccccccccccc} 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \end{array}\right]^\top,$$
$$\frac{1}{5}\left[\begin{array}{cccccccccccccccccc} 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \end{array}\right]^\top,$$
$$\frac{1}{5}\left[\begin{array}{cccccccccccccccccc} 1 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 \end{array}\right]^\top.$$

Applying Proposition 3.4, it can be verified that for each $j = 1, \dots, 4$, $diag(c_j)$ is an extreme point of Δ.

Note that the positive vector x given below is a solution to the linear system $\left[\begin{array}{c} A \\ \hline comp(A) \end{array}\right] x = \left[\begin{array}{c} \mathbf{1}_6 \\ \hline \frac{3}{5}\mathbf{1}_{15} \end{array}\right]$:

$$x = \frac{1}{20}\left[\begin{array}{cccccccccccccccccc} 3 & 3 & 3 & 3 & 2 & 2 & 2 & 2 & 4 & 1 & 1 & 1 & 1 & 4 & 2 & 2 & 2 & 2 \end{array}\right]^\top.$$

Further, it turns out that the null space of $\left[\begin{array}{c} A \\ \hline comp(A) \end{array}\right]$ is spanned by the columns of the matrix

$$Z = \left[\begin{array}{ccc} -1 & -1 & -1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & -1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 1 \end{array}\right].$$

Hence, Δ can be described as $\Delta = \{diag(y) | y \geq 0, y = Zu + x \text{ for some } u \in \mathbb{R}^3\}$. In particular, if u is such that $Zu + x \geq 0$, then by considering the 10–th through 13–th entries of the inequality $Zu + x \geq 0$, we find that

$$u_1 + u_2 \leq \frac{1}{20}, u_1 + u_3 \leq \frac{1}{20}, u_1 + u_2 + u_3 \geq -\frac{1}{20} \text{ and } u_1 \geq -\frac{1}{20}. \tag{14}$$

Let C be the 18×4 matrix whose columns are (in order) $c_1, \ldots, c_4$, and suppose that we have a vector $u \in \mathbb{R}^3$ such that $Zu + x \geq 0$. Solving the linear system $Cv = Zu + x$, we find that

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} -5 & -5 & 0 \\ -5 & 0 & -5 \\ 5 & 5 & 5 \\ 5 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} + \frac{1}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

From the inequalities (14) we find that $v_j \geq 0, j = 1, \ldots, 4$, and it is readily seen that $\sum_{j=1}^{4} v_j = 1$. Hence, for any u such that $Zu + x \geq 0$, we may write $Zu + x$ as a convex combination of the vectors $c_1, \ldots, c_4$. We now deduce that Δ is the convex hull of the matrices $diag(c_1), \ldots, diag(c_4)$.

It is straightforward to see that an $n \times m$ $(0, 1)$ matrix A with exactly one 0 in each column, and no row (respectively, column) dominated by another row (respectively, column), can be brought to the form $J_n - I_n$ by row and column permutations, in which case $(A, \frac{1}{n-1} I_n)$ is a mock design. Our next goal is to consider $(0, 1)$ matrices having two 0s in each column that lead to mock designs. To that end, we consider the sequence of $n \times \binom{n}{2}$ matrices $B(n)$ constructed iteratively as follows:

$$B(3) = I_3, B(l+1) = \left[\begin{array}{c|c} 0_l^\top & \mathbf{1}_{\binom{l}{2}}^\top \\ \hline J_l - I_l & B(l) \end{array}\right], l \geq 3.$$

Suppose that $n \geq 3$, and that A is a $(0, 1)$ matrix with n rows having two 0s in each column. We note that necessarily the columns of A must be selected from those of $B(n)$.

Lemma 3.3. *For each $l \geq 3$, the $\binom{l+1}{2} \times \binom{l}{2}$ matrix $\left[\begin{array}{c} B(l) \\ \hline comp(B(l)) \end{array}\right]$ has rank $\binom{l}{2}$.*

Proof. We proceed by induction on l and note that the case $l = 3$ is readily established. Suppose that the assertion holds for some $l \geq 3$, and observe that

$$\left[\begin{array}{c} B(l+1) \\ \hline comp(B(l+1)) \end{array}\right] = \left[\begin{array}{c|c} 0_l^\top & \mathbf{1}_{\binom{l}{2}}^\top \\ \hline J_l - I_l & B(l) \\ \hline 0 & B(l) \\ \hline comp(J_l - I_l) & comp(B(l)) \end{array}\right].$$

Let $\left[\begin{array}{c} x \\ \hline y \end{array}\right]$ be a null vector for $\left[\begin{array}{c} B(l+1) \\ \hline comp(B(l+1)) \end{array}\right]$. Then $(J_l - I_l)x + B(l)y = 0$ and $B(l)y = 0$; since $l \geq 3$, $J_l - I_l$ is nonsingular, so we find that $x = 0$. But then y is a null vector for $\left[\begin{array}{c} B(l) \\ \hline comp(B(l)) \end{array}\right]$, and applying the induction hypothesis, we see that

y must be 0. Hence $\left[\dfrac{B(l+1)}{comp(B(l+1))}\right]$ has nullity zero, which completes the proof of the induction step.

$\square$

Theorem 3.5. *Let A be an $n \times m$ $(0,1)$ matrix with distinct columns and two 0s in each column. There is a diagonal matrix D with nonnegative diagonal entries such that (A, D) is a mock design if and only if, up to row and column permutations, $A = B(n)$. In that case, necessarily $D = \frac{2}{(n-1)(n-2)} I$.*

Proof. Suppose first that (A, D) is a mock design for some nonnegative diagonal matrix D. We assume without loss of generality that A has no repeated columns. Each nonzero column of A is necessarily a column of $B(n)$. Hence, it follows that (by adding some zero diagonal entries if necessary) we may extend D to a diagonal matrix $\widehat{D}$ of order $\binom{n}{2}$ so that for a suitable permutation matrix P we have $B(n)\widehat{D}P = \left[\begin{array}{c|c} AD & 0 \end{array}\right]$. Since $ADA^\top = \frac{2}{n-1} I + \frac{n-3}{n-1} J$, we see that the vector $\widehat{D}\mathbf{1}$ is a solution to the following linear system:

$$\left[\frac{B(n)}{comp(B(n))}\right] x = \left[\frac{\mathbf{1}_n}{\frac{n-3}{n-1}\mathbf{1}_{\binom{n-1}{2}}}\right]. \tag{15}$$

From Lemma 3.3, we find that the coefficient matrix of (15) has full column rank. Noting that $x = \frac{1}{\binom{n-1}{2}} \mathbf{1}_{\binom{n}{2}}$ is the solution to (15), we thus conclude that $\widehat{D} = \frac{2}{(n-1)(n-2)} I_{\binom{n}{2}}$ and that $A = B(n)P$. The converse is straightforward. $\square$

Suppose that we are given a $(0,1)$ matrix A with constant column sums, a diagonal matrix D such that (A, D) is a mock design, and suppose further that D is an extreme point of the set Δ. From Proposition 3.4 it follows that the vector consisting of the nonzero diagonal entries of D is the solution to a linear system whose coefficient matrix is $(0,1)$ and has full column rank, and whose right–hand sides are all rational numbers. In particular, we find that the diagonal entries of D must all be rational. Our final result gives more insight into the structure of A in that setting, and makes another connection between mock designs and balanced incomplete block designs.

Theorem 3.6. *Let A be an $n \times m$ $(0,1)$ matrix with $c \geq 1$ 0s in each column. Suppose that D is a diagonal matrix of order m such that each diagonal entry is positive and rational, write D as $D = \frac{1}{q} diag(p)$, where $q, p_1, \ldots, p_m \in \mathbb{N}$. Then (A, D) is a mock design if and only if the matrix B given by*

$$B = \left[\begin{array}{c|c|c|c} Ae_1\mathbf{1}_{p_1}^\top & Ae_2\mathbf{1}_{p_2}^\top & \ldots & Ae_m\mathbf{1}_{p_m}^\top \end{array}\right] \tag{16}$$

is the incidence matrix of a balanced incomplete block design with parameters $(v, k, \lambda) = (n, n-c, \frac{q(n-c-1)}{n-1})$.

Proof. Suppose first that (A, D) is a mock design, so that $ADA^\top = \frac{c}{n-1}I+(1-\frac{c}{n-1})J$. Hence we have $\sum_{l=1}^m a_{i,l}d_l a_{i,l} = 1, i = 1,\ldots,n$, and $\sum_{l=1}^m a_{i,l}d_l a_{j,l} = \frac{n-c-1}{n-1}$, for $1 \le i < j \le n$. Since $d_l = \frac{p_l}{q}$ for each $l = 1,\ldots,m$, we see that $\sum_{l=1}^m a_{i,l}^2 p_l = q, i = 1,\ldots,n$, and $\sum_{l=1}^m a_{i,l}p_l a_{j,l} = \frac{q(n-c-1)}{n-1}$, for $1 \le i < j \le n$. Set $s = \sum_{l=1}^m p_l$. Referring to (16), we see that these last two conditions are equivalent to $\sum_{l=1}^s b_{i,l}^2 = q, i = 1,\ldots,n$, and $\sum_{l=1}^s b_{i,l}b_{j,l} = \frac{q(n-c-1)}{n-1}$, for $1 \le i < j \le n$, respectively. Consequently $BB^\top = \frac{qc}{n-1}I+\frac{q(n-c-1)}{n-1}J$, so that B is a the incidence matrix of a balanced incomplete block design with parameters $(n, n-c, \frac{q(n-c-1)}{n-1})$. The converse is straightforward. $\square$

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