

Maximum Determinant of (0,1) Matrices with Constant Line Sums

by

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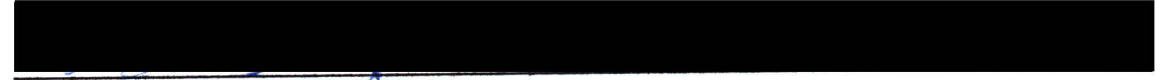
MASTER OF SCIENCE


in the Department of Mathematics and Statistics

We accept this thesis as conforming
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Abstract


The maximum absolute value of the determinant of $n \times n$ nonsingular $(0,1)$ matrices that have constant row and column sums k is investigated. Recently the minimum absolute value of the determinant for matrices in this class has been proved to be $k \gcd(n, k)$ for all $(n, k) \neq (4, 2)$. However, there appears to be no such general formula for the maximum determinant. For $n \neq 4$, $k = 2$, the maximum determinant is proved to be 2^t if $n = 3t$ or $3t + 2$, and 2^{t-1} if $n = 3t + 1$. Restriction to a subset of these matrices, namely those that are symmetric and have zero trace (their graphs are regular of degree k), leaves this minimum and maximum unchanged for $k = 2$. For this restricted class, when $n \geq 7$, $k = n - 3$, the minimum again remains unchanged and the maximum absolute value of the determinant is $(n - 3)3^{\lfloor n/4 \rfloor - 1}$. This maximum gives a lower bound for the maximum absolute value of the determinant of the larger class, but in general this bound is not tight. Other determinantal values and bounds for specific n and k are derived. For reference a table is given of presently known values of the minimum and maximum absolute value of the determinant of $n \times n$ nonsingular $(0,1)$ matrices with constant row and column sums k , and of the associated restricted class. In addition to evaluation of the maximum absolute value of the determinant, matrices are exhibited that attain these maximum values. Additional relationships are shown to exist between $n \times n$ nonsingular $(0,1)$ matrices that have constant row and column sums 2, and the associated restricted class. A localization result is established for the subdominant eigenvalues for the matrices in the restricted class.

Examiners


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Dedication

This thesis is dedicated to
my parents, for their
unfailing support and
encouragement throughout my life.

Introduction

In this thesis the problem of maximizing the absolute value of the determinant of nonsingular $(0,1)$ matrices with constant row and column sums is discussed. The discussion is aimed at a reader who is familiar with basic facts about linear algebra, matrix theory and graph theory.

Background and History

The problem of maximizing the determinant of certain families of matrices has been studied extensively. One of the classical bounds is Hadamard's bound for positive semi-definite matrices (see Theorem 1.2.3). Analysis of this bound leads to the study of matrices known as Hadamard matrices, see, for example, [15], [19]. Cheng [5] and Cheng *et al.* [6] were interested in maximizing the determinant of a restricted class of positive semi-definite matrices, known as Laplacian matrices. This maximization problem is equivalent to maximizing the number of spanning trees in a connected graph, which, as stated in [5], has applications in network reliability and statistics.

We now turn our attention to $(0,1)$ matrices, where $(0,1)$ matrices are defined to be matrices in which each entry is either zero or one. In 1956, Ryser [18] proved a re-

markable theorem (see Theorem 1.2.6) that motivates maximizing the determinant of $(0,1)$ matrices. Williamson [22] was concerned with the connections between the problems of maximizing the determinant of matrices with ± 1 entries and $(0,1)$ matrices. Williamson [22] established that the maximum determinant of an $n \times n$ (± 1) matrix is equal to 2^{n-1} times the maximum determinant of an $(n-1) \times (n-1)$ $(0,1)$ matrix. With our restriction of constant row and column sums placed on $(0,1)$ matrices, this bound is of little use. Brualdi and Solheid [3] were interested in maximizing the determinant of $(0,1)$ matrices whose zeros form an acyclic pattern.

In 1970, Newman [16] discussed determinantal results specifically concerning the set of all $n \times n$ $(0,1)$ matrices with constant row and column sums k , where $1 \leq k \leq n-1$. A matrix with constant row and column sums k is said to have constant line sums k . Newman [16] established that this set contains nonsingular matrices for all n, k with one exception when $n = 4, k = 2$. Thus it is reasonable to consider the extremum of the determinant of nonsingular matrices in this set. Newman [16] conjectured that the minimum positive determinant in this set is $k \cdot \gcd(n, k)$, for $(n, k) \neq (4, 2)$. Later Grady [9] also considered minimizing the absolute value of the determinant of $n \times n$ nonsingular $(0,1)$ matrices with constant line sums k . He described an algorithm for constructing matrices that obtained this minimum positive determinant, and used this algorithm to numerically verify Newman's conjecture for several thousand cases with $n \leq 90$. In 1995, Li *et al* [14]

proved Newman's conjecture for the minimum positive determinant for all n, k (see Theorem 1.4.1). Specifically, Li *et al.* [14] verified Grady's algorithm for $(n, k) = (6, 2)$ and $n = 2k$. They then constructed $n \times n$ nonsingular $(0, 1)$ matrices with constant line sums k for other choices of (n, k) , with determinant $k \cdot \gcd(n, k)$, by using a Schur complement technique along with some of the results in [16]. Grady and Newman [10] have very recently presented a proof that Grady's algorithm [9] holds in general.

Hence we are concerned with maximizing the absolute value of the determinant of nonsingular $(0, 1)$ matrices with constant line sums. Although Newman was interested in minimizing the determinant, he gave basic results pertaining to the determinant of such matrices, which we exploit throughout.

Main Purpose of the Thesis

This thesis presents results on the maximum absolute value of the determinant of an $n \times n$ nonsingular $(0, 1)$ matrix with fixed constant line sums k , $1 \leq k \leq n - 1$, for $n \geq 2$. The motivation for this came from a recent proof of a formula for the minimum absolute value of the determinant for this set. As some classical upper bounds are known, we determine lower bounds and formulae in general. To derive lower bounds we consider a subset of these matrices, namely the set of all $n \times n$ symmetric, nonsingular $(0, 1)$ matrices with zero trace and constant line sums k .

These are related to finite regular graphs of degree k . Employing results from graph theory aids in constructing lower bounds, or in particular cases gives general formulae for the maximum absolute value of the determinant for the subset. The minimum absolute value of the determinant for the subset is also considered.

Organization of the Thesis

In Chapter 1, we discuss basic definitions and notation related to the problem of maximizing the absolute value of the determinant of a nonsingular $(0,1)$ matrix with constant line sums, and give some immediate consequences. We include some of the results of Newman [16] and reprove some of these as our definitions are slightly different. We give a concise survey of other related results. Our analysis utilizes techniques from graph theory and combinatorics, thus we state a few standard definitions and results from these areas. Specific examples are given to clarify some of the introductory techniques developed.

In Chapter 2, we consider the problem of maximizing the absolute value of the determinant of $n \times n$ nonsingular $(0,1)$ matrices with constant line sums 2. In this case we derive a formula for the maximum as a function of n . Our first step is to describe a canonical form for $n \times n$ nonsingular $(0,1)$ matrices with constant line sums 2. We show that every such matrix is permutationally equivalent to a block diagonal matrix where each block has the same $(0,1)$ pattern, but the blocks may vary in

size. This reduces our study to these block matrices. From our analysis we derive a recurrence relation involving the maximum absolute value of the determinant in this case, thus determining the formula for this maximum.

Since the corresponding values for $n \times n$ nonsingular $(0,1)$ matrices with constant line sums 2 are known, the determination of the maximum and the minimum determinant of absolute value of the $n \times n$ symmetric, nonsingular $(0,1)$ matrices with zero trace and constant line sums 2 is now less complicated. However, we also derive a canonical form for the matrices in this restricted class. Using the restriction of symmetry and zero trace, we show that every such matrix is permutationally similar to another block diagonal matrix.

In Chapter 3, we consider another restricted class, namely $n \times n$ symmetric, nonsingular $(0,1)$ matrices with zero trace and constant line sums $n - 3$. We derive general formulae for the minimum and for the maximum absolute value of the determinant of such matrices using the canonical form described in Chapter 2. This then gives rise to lower bounds for the maximum absolute value of the determinant of the larger classes of $n \times n$ nonsingular $(0,1)$ matrices with constant line sums 3 and $n - 3$.

In the final chapter we supply a few independent but related results. We prove that in the case n odd there are additional relationships between $n \times n$ symmetric, nonsingular $(0,1)$ matrices with zero trace and constant line sums 2, and $n \times n$

nonsingular $(0,1)$ matrices with constant line sums 2. We establish that in order for this relationship to hold it is also sufficient that n is odd. This relationship gives rise to a method for computing the eigenvalues of a certain class of real tridiagonal matrices. We also give a localization result on the subdominant eigenvalues of $n \times n$ symmetric, nonsingular $(0,1)$ matrices with zero trace and constant line sums k . We conclude by summarizing the main results of the thesis, and present a table of presently known values for the extrema of the absolute value of the determinants for the two classes of matrices described above. In addition, we show open problems that remain.

Chapter 1

Definitions and Preliminary Results

In this chapter we give some definitions that are related to the problem of maximizing the absolute value of the determinant of nonsingular $(0,1)$ matrices with constant line sums (that is, constant row and column sums). We also elaborate on the results briefly mentioned in the Introduction.

1.1 Basic Facts and Notation

We begin by reviewing some basic facts and notation that are used throughout. For more definitions and facts about matrices and linear algebra, see [13]. Let \mathbf{R} , \mathbf{R}^+ , and \mathbf{Z} denote the set of real numbers, positive real numbers, and integers, respectively. Let $a_{ij} \in \mathbf{R}$. Then $A = [a_{ij}] \in M_n$ is an $n \times n$ real *matrix* with entries a_{ij} . Let I_n and J_n denote the $n \times n$ identity and the matrix of all ones, respectively, the subscript is dropped when the order is clear from the context. Let e denote the $n \times 1$ vector of all ones, and A^T denote the *transpose* of A . It is easy to see that $J_n = ee^T$. Let $\text{tr} A$ denote the *trace* of A , which is defined to be $\sum_{i=1}^n a_{ii}$.

The determinant of A , denoted $\det A$, is defined to be

$$\det A = \sum_{\sigma \in S_n} \operatorname{sgn} \sigma \prod_{i=1}^n a_{i\sigma(i)},$$

where S_n denotes the symmetric group on n elements. An equivalent definition of the determinant is known as the Laplace expansion of the determinant. Using this definition,

$$\det A = \sum_{i=1}^n (-1)^{i+j} a_{ij} \det(A(i, j)) = \sum_{j=1}^n (-1)^{i+j} a_{ij} \det(A(i, j)),$$

for all $1 \leq i, j \leq n$, where $A(i, j)$ is the $(n-1) \times (n-1)$ submatrix obtained from A by deleting row i and column j .

Note that the determinant is a multilinear function acting on $n \times n$ matrices. If A is an $n \times n$ matrix and A' is obtained from A by interchanging two rows (columns), then $\det A' = -\det A$. If A' is obtained from A by adding a scalar multiple of any one row (column) to another row (column), then $\det A' = \det A$. These results are easy to prove using the Laplace expansion of the determinant and can be found in [13]. The *characteristic polynomial* of A is by definition $\det(\lambda I - A)$, where λ is a scalar. We denote the characteristic polynomial of A by $p_A(\lambda)$. If A is an $n \times n$ matrix, then an *eigenvalue* of A is a root of $p_A(\lambda) = 0$. Equivalently, λ is a complex number such that $Ax = \lambda x$, where x is an $n \times 1$ nonzero vector. It is an easy induction argument to show that $\det A = \prod_{i=1}^n \lambda_i$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of A .

For $n \geq 2$ and k an integer, let $S(n, k)$ denote the set of all $n \times n$ nonsingular $(0,1)$ matrices with all line sums equal to k ($1 \leq k \leq n-1$). In the Introduction we stated that Newman [16] showed that $S(n, k) \neq \phi$ for all n, k with the one exception when $n = 4$ and $k = 2$. We discuss this fact in more detail in Chapter 2. Also note that our set $S(n, k)$ does not include singular matrices, cf. [14], [16]. We let

$$M(n, k) = \max\{|\det A| : A \in S(n, k)\}, \text{ and } m(n, k) = \min\{|\det A| : A \in S(n, k)\}.$$

We consider a subset of $S(n, k)$ that is in one to one correspondence with a special class of finite graphs. A *graph* $G = (V, E)$ has (finite) vertex set V and edge set E where E is a subset of the unordered pairs of V . All graphs considered here have no multiple edges or loops. For more definitions and facts concerning graph theory, see [21]. If $V_1 \cap V_2 \neq \phi$, $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, then $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. If $A = [a_{ij}]$ is an $n \times n$ symmetric entry-wise non-negative matrix with zero trace, then the *graph of* A , denoted $G(A)$, has vertex set $V = \{1, 2, \dots, n\}$ and $\{i, j\} \in E$ if and only if $i \neq j$ and $a_{ij} = a_{ji} \neq 0$. If G is any graph, then $A(G) = [a_{ij}]$ is called the *adjacency matrix of* G if $a_{ij} = a_{ji} = 1$ whenever $i \neq j$ and $\{i, j\} \in E$, and $a_{ij} = a_{ji} = 0$ otherwise. The *degree* of a vertex v in G , denoted by $\text{deg}(v)$, is the number of edges incident with v . A graph G is *regular* of degree k if every vertex in G has degree k . A graph G with $V = \{x_1, x_2, \dots, x_n\}$ is an *n -cycle*, $n \geq 2$, denoted by C_n , if its edges consist exactly of $\{x_n, x_1\}$, and $\{x_i, x_{i+1}\}$ for $1 \leq i \leq n-1$. Let $G(n, k) \subset S(n, k)$ denote the set of all nonsingular

$n \times n$ symmetric $(0,1)$ matrices with all line sums k and zero trace. We let

$$W(n, k) = \max\{|\det A| : A \in G(n, k)\}, \text{ and } w(n, k) = \min\{|\det A| : A \in G(n, k)\}$$

If $A \in G(n, k)$, then $G(A)$ is a graph on n vertices that is regular of degree k , with adjacency matrix A (up to permutation similarity). Also if $A \in G(n, k)$, then $kI - A$ is a Laplacian matrix of $G(A)$. We noted that $S(n, k) \neq \phi$ for all n, k with one exception when $n = 4, k = 2$. However, this is not the case for $G(n, k)$. It is a simple combinatorial argument to verify that $\sum_{v \in V} \deg(v) = 2|E|$, hence the number of vertices with odd degree must be even, whence if both n, k are odd, then $G(n, k) = \phi$. Additionally, if $A \in G(n, n-2)$, then there exists an $i \neq 1$ so that $a_{1,i} = 0$ hence $a_{i,1} = 0$, and since $a_{1,1} = a_{i,i} = 0$, row 1 and row i are identical. Thus $G(n, n-2) = \phi$. For other values of n, k , it is also possible that $G(n, k)$ is empty, for example $G(6, 3) = \phi$; see Example 1.4.7. If for a given n and k with $1 \leq k \leq n-1$, $G(n, k) \neq \phi$, then, since $G(n, k) \subset S(n, k)$, it follows that

$$0 < m(n, k) \leq w(n, k) \leq W(n, k) \leq M(n, k)$$

The above inequalities are useful in many propositions

1.2 Classical Upper bounds for $M(n, k)$

We begin by discussing some well known upper bounds for $M(n, k)$. If $A \in S(n, k)$, then A is a $(0,1)$ matrix and hence an entry-wise nonnegative matrix. Entry-wise

nonnegative matrices have been studied extensively (see, for example, [2]). One of the well known results is the Perron-Frobenius Theorem (see [2], [13]). The *spectral radius* of A , denoted by $\rho(A)$, is defined to be

$$\rho(A) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } A\}$$

It is well known that for any matrix norm $\|\cdot\|$,

$$\rho(A) = \lim_{k \rightarrow \infty} \|A^k\|^{1/k},$$

(see [13] p. 299) Some examples of matrix norms are

$$\|A\|_2 = \left(\sum_{i,j} |a_{ij}|^2 \right)^{1/2} \quad \text{and} \quad \|A\|_\infty = \max_{1 \leq i \leq n} \left(\sum_{j=1}^n |a_{ij}| \right)$$

It follows easily that $\rho(A) \leq \|A\|$ for any matrix norm $\|\cdot\|$. Using the limit relation above and the $\|\cdot\|_2$ norm, it can be shown that if A, B are entry-wise nonnegative matrices and $A - B$ is an entry-wise nonnegative matrix, then $\rho(A) \geq \rho(B)$. We state the following version of the Perron-Frobenius theorem (see [13] p. 503).

THEOREM 1.2.1 (Perron-Frobenius) *If A is an $n \times n$ entry-wise nonnegative matrix, then $\rho(A)$ is an eigenvalue of A , and there is an entry-wise nonnegative vector $x \neq 0$ such that $Ax = \rho(A)x$*

PROPOSITION 1.2.2 *If $A = [a_{ij}]$ is an $n \times n$ entry-wise nonnegative matrix, then for $1 \leq i \leq n$*

$$\min_i \left(\sum_{j=1}^n a_{ij} \right) \leq \rho(A) \leq \max_i \left(\sum_{j=1}^n a_{ij} \right)$$

Proof. If $\min_i (\sum_{j=1}^n a_{ij}) = 0$, then the result is trivial. Suppose $\min_i (\sum_{j=1}^n a_{ij}) = \alpha \neq 0$, then let $B = [b_{ij}]$, where $b_{ij} = \alpha a_{ij} / (\sum_{j=1}^n a_{ij}) \leq a_{ij}$. Then $A - B$ is entry-wise non-negative, and so $\rho(B) \leq \rho(A)$. However, $\rho(B) \leq \|B\|_\infty = \alpha \leq \rho(B)$, as $Be = \alpha e$. Hence $\rho(B) = \alpha$, therefore $\rho(A) \geq \alpha$. Similar arguments can be applied to the maximum as well. \square

If $A \in S(n, k)$, then $\rho(A) = k$ with a corresponding eigenvector e . Hence if $A \in S(n, k)$, then

$$|\det A| \leq M(n, k) \leq k^n$$

However, for $k \geq 2$ this bound is not tight for $A \in S(n, k)$.

The following theorem is known as Hadamard's inequality and can be found in [13] p. 477. An $n \times n$ matrix A is *positive semi-definite* if $x^T A x \geq 0$ for all $n \times 1$ real vectors x .

THEOREM 1.2.3 (Hadamard) *If $A = [a_{ij}]$ is an $n \times n$ positive semi-definite matrix, then*

$$|\det A| \leq \prod_{i=1}^n a_{ii}$$

Equality holds if and only if A is a diagonal matrix

If A is an $n \times n$ matrix, then it is easy to see that AA^T is an $n \times n$ positive semi-definite matrix. This follows since $x^T AA^T x$ is equal to the square of the Euclidean

length of the real vector $A^T x$, and hence is nonnegative. This observation together with Theorem 1 2 3 gives the following corollary

COROLLARY 1 2.4 (Hadamard) *If $A = [a_{ij}]$ is an $n \times n$ matrix, then*

$$|\det A| \leq \prod_{i=1}^n \left(\sum_{j=1}^n a_{ij}^2 \right)^{1/2}$$

Proof. The i th diagonal entry of AA^T is $\sum_{j=1}^n a_{ij}^2$, and since $(\det A)^2 = \det(AA^T)$, the result follows using Theorem 1 2 3. \square

If $A \in S(n, k)$, then for $i = 1, 2, \dots, n$, $\sum_{j=1}^n a_{ij}^2 = k$, and by Corollary 1 2 4

$$|\det A| \leq M(n, k) \leq k^{n/2}$$

Note that this is a sharper upper bound than the one obtained by using the Perron-Frobenius theorem. Equality holds in Corollary 1 2 4 if and only if AA^T is diagonal, that is, if and only if A has orthogonal row vectors (hence $|\det A| = k^{n/2}$ if and only if A has orthogonal rows). Since A is also a $(0,1)$ matrix, no row or column of A can have more than one nonzero entry. Hence $A = Q$, where Q is a *permutation matrix*, which by definition is an $n \times n$ $(0,1)$ matrix such that $QQ^T = Q^TQ = I_n$. Thus Hadamard's bound is never attained for $A \in S(n, k)$, when $k \geq 2$.

Before discussing our next and final classical upper bound, we begin with some basic definitions and facts from combinatorial design theory. For a comprehensive

reference concerning combinatorial mathematics, see [19]. Let T be a ν -set with elements x_1, x_2, \dots, x_ν . Let T_1, T_2, \dots, T_ν be ν subsets of T . Then T_1, T_2, \dots, T_ν is a (ν, k, λ) -*configuration* if the following hold

- (i) $|T_i| = k$ for all $1 \leq i \leq \nu$,
- (ii) $|T_i \cap T_j| = \lambda$ for all $1 \leq i \neq j \leq \nu$, and
- (iii) $0 < \lambda < k < \nu$

For $1 \leq i, j \leq \nu$, let $a_{ij} = 1$ if $x_j \in T_i$, and 0 otherwise. Then the $\nu \times \nu$ matrix $A = [a_{ij}]$ is called the *incidence matrix* of the (ν, k, λ) -configuration. By (i) and (ii) it follows that

$$AJ = kJ, \text{ and } AA^T = (k - \lambda)I + \lambda J.$$

By (iii) and the equation above, it follows that A is nonsingular. Using the equations above, $JAJ = kJ^2 = k\nu J$, and $AA^T J = (k - \lambda + \nu\lambda)J$. Since A is nonsingular, $A^T J = (k - \lambda + \nu\lambda)A^{-1}J$. Taking the transpose of both sides and using the fact that $A^{-1}J = (1/k)J$, gives $JA = ((k - \lambda + \nu\lambda)/k)J$. Therefore $JAJ = (\nu(k - \lambda + \nu\lambda)/k)J$. From above this means that

$$k\nu = (k - \lambda + \nu\lambda)\nu/k.$$

Hence there is a relationship between λ , ν and k , namely

$$\lambda = k(k - 1)/(\nu - 1).$$

In order to find the determinant of an incidence matrix we give the following general lemma. Using the Jordan canonical form theorem (see [13] p. 126), it is easy to see that the rank of an $n \times n$ matrix A is an upper bound for the number of nonzero eigenvalues (counting multiplicities) of A . This lemma is well known (see, for example, [17]).

LEMMA 1.2.5 *Let B be an $n \times n$ rank one matrix. Then*

$$\det(I + B) = 1 + \operatorname{tr} B$$

Proof. Since B is a real $n \times n$ rank one matrix, by the remarks above, there exists at most one nonzero eigenvalue of B , say λ_1 . It is a well known fact that $\sum_{i=1}^n \lambda_i = \operatorname{tr} B$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of B , see [13] p. 42. Hence $\operatorname{tr} B = \lambda_1$, as $\lambda_j = 0$ for $2 \leq j \leq n$. If λ is an eigenvalue of B , then $1 + \lambda$ is an eigenvalue of $I + B$. Therefore,

$$\det(I + B) = \prod_{i=1}^n (1 + \lambda_i) = 1 + \lambda_1 = 1 + \operatorname{tr} B. \quad \square$$

Using Lemma 1.2.5 it follows that, for $a, b \in \mathbf{R}$, $\det(aI_n + bJ_n) = a^{n-1}(a + nb)$

Thus, if A is the incidence matrix of a (ν, k, λ) -configuration, then

$$|\det A| = (\det((k - \lambda)I + \lambda J))^{1/2},$$

$$\begin{aligned}
&= \left((k - \lambda + \nu\lambda)(k - \lambda)^{\nu-1} \right)^{1/2}, \\
&= k(k - \lambda)^{(\nu-1)/2},
\end{aligned}$$

by using the above formula for λ . Note that above we have also shown that $JA = kJ$, hence if A is the incidence matrix of a (ν, k, λ) -configuration, then $A \in S(\nu, k)$. The next theorem due to Ryser [18] deals specifically with $(0,1)$ matrices and gives some motivation for maximizing the absolute value of the determinant of $(0,1)$ matrices.

THEOREM 1.2.6 (Ryser) *For $n \geq 2$, let A be an $n \times n$ $(0,1)$ matrix with a total of t ones. Set $k = t/n$ and $\lambda = k(k - 1)/(n - 1)$, and suppose that $0 < \lambda < k < n$. Then $|\det A| \leq k(k - \lambda)^{(n-1)/2}$, with equality holding if and only if A is the incidence matrix of a (n, k, λ) -configuration.*

Thus Theorem 1.2.6 gives another upper bound for $M(n, k)$, namely

$$M(n, k) \leq k(k - \lambda)^{(n-1)/2},$$

where $\lambda = k(k - 1)/(n - 1)$. Equality holds if and only if A is the incidence matrix of a (n, k, λ) -configuration. If the parameters n, k, λ admit a (n, k, λ) -configuration, then $M(n, k)$ is determined, see Example 1.4.5. However, since it is required that $\lambda \in \mathbf{Z}$ and positive, there are infinitely many values of n, k for which there does not exist a (n, k, λ) -configuration, so in general this bound is not tight.

If a $(s^2 + s + 1, s + 1, 1)$ -configuration exists, it is called a *projective plane of order s* . It is well known (see [19] p. 93) that if $s = p^\alpha$, where p is a prime number and $\alpha \geq 1$ an integer, then there exists a projective plane of order s . In this case,

$$M(s^2 + s + 1, s + 1) = (s + 1)s^{(s^2+s)/2}$$

For example, $M(13, 4) = 2916$.

1.3 $Z(n, k)$ and $Z_+(n, k)$

For completeness we consider two sets related to $S(n, k)$. Take $n \geq 2$ and $k \in \mathbf{Z}$. Let $Z(n, k)$ denote the set of all $n \times n$ integer matrices with all line sums equal to k , for $k \neq 0$. Similarly let $Z_+(n, k)$ denote the set of all $n \times n$ nonnegative integer matrices with all line sums equal to k , for $k \geq 1$. We state the results for the minimum positive determinants in $Z(n, k)$ and $Z_+(n, k)$ as established in [14] Th 2

THEOREM 1.3.1 *Let $n \geq 2$ and k be nonzero integers*

(a) *Then $\min\{|\det A| : A \in Z(n, k), \det A \neq 0\} = |k| \cdot \gcd(n, k)$*

(b) *If $k \geq 1$, then $\min\{|\det A| : A \in Z_+(n, k), \det A \neq 0\} = k \cdot \gcd(n, k)$*

We give the following general lemma to aid the proof of the next theorem.

LEMMA 1.3.2 *Suppose $x_i \in \mathbf{R}^+ \cup 0$, and $\sum_{i=1}^n x_i = k$. Then $\sum_{i=1}^n x_i^2 \leq k^2$, with equality holding if and only if there is a unique j : $1 \leq j \leq n$, so that $x_j = k$ and $x_i = 0$ for $i \neq j$.*

Proof. Since each $x_i \geq 0$,

$$\left(\sum_{i=1}^n x_i \right)^2 = \sum_{i=1}^n x_i^2 + \sum_{i \neq j} x_i x_j \geq \sum_{i=1}^n x_i^2.$$

Therefore $\sum_{i=1}^n x_i^2 \leq k^2$. Equality holds if and only if $\sum_{i \neq j} x_i x_j = 0$. Also since each $x_i \geq 0$, there can exist at most one x_j nonzero. Hence, since $\sum_{i=1}^n x_i = k$, it follows that there exist a unique j so that $x_j = k$ and $x_i = 0$ for $i \neq j$. \square

Now to determine $\sup\{|\det A| : A \in Z(n, k)\}$ and $\max\{|\det A| : A \in Z_+(n, k)\}$ is not difficult.

THEOREM 1.3.3 *Let $n \geq 2$ and k be nonzero integers. Then $\sup\{|\det A| : A \in Z(n, k)\}$ is unbounded, and $\max\{|\det A| : A \in Z_+(n, k)\} = k^n$.*

Proof. Let $x \in \mathbf{Z}$, and let

$$B = \begin{bmatrix} k & k-x & 0 & \cdots & 0 & x-k \\ 0 & x & k-x & 0 & \cdots & 0 \\ 0 & 0 & x & k-x & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & x & k-x \\ 0 & 0 & \cdots & 0 & 0 & k \end{bmatrix} \quad (1.1)$$

Then $B \in Z(n, k)$ and $|\det B| = k^2|x|^{n-2}$, since B is upper triangular. Thus $\sup\{|\det A| : A \in Z(n, k)\} \geq k^2|x|^{n-2}$, and this inequality holds for every $x \in \mathbf{Z}$. Hence $\sup\{|\det A| : A \in Z(n, k)\}$ is unbounded. However, if B as in (1.1) were in $Z_+(n, k)$, then $x = k$, and therefore $|\det B| = k^n$. Using Lemma 1.3.2 and Corollary 1.2.4 implies that $\max\{|\det A| : A \in Z_+(n, k)\} = k^n$. This proves the desired result. \square

1.4 Basic Propositions and Examples

In this section we discuss some more basic results concerning matrices in $S(n, k)$ and $G(n, k)$, and we denote $\gcd(n, k)$ by d . For reference, we state here the theorem evaluating $m(n, k)$ discussed in the Introduction, and proved in [14]

THEOREM 1.4.1 For $n = 3$ and $n \geq 5$,

$$m(n, k) = kd.$$

The next proposition restricts the values of the determinant of matrices in $S(n, k)$. This proposition can be found in [16]. We present a proof here for completeness.

PROPOSITION 1.4.2 *If $A \in S(n, k)$, then kd divides $|\det A|$.*

Proof. Add rows $2, 3, \dots, n$ to row 1. The resulting matrix A' has first row $[k, k, \dots, k]$. Hence $|\det A| = |\det(A')| = k|\det(A'')|$, where A'' has rows $2, 3, \dots, n$ the same as A , and row 1 is e^T . Now add columns $2, 3, \dots, n$ to column 1. The resulting matrix A''' has first column $[n, k, \dots, k]^T$, from which we can factor out d , resulting in $A^{(w)}$. Thus

$$|\det A| = k|\det(A'')| = k|\det(A''')| = kd|\det(A^{(w)})|$$

Since $A^{(w)}$ has integer entries, $\det(A^{(w)}) \in \mathbf{Z}$. Thus kd divides $|\det A|$. \square

The following result was given by Newman [16]. We present a different proof here.

PROPOSITION 1.4.3 *If $A \in S(n, k)$, then*

$$\det(J - A) = (-1)^{n-1} \binom{n-k}{k} \det A$$

Proof Since $A \in S(n, k)$, A^{-1} exists. Thus

$\det(J - A) = (-1)^n \det A \cdot \det(I - JA^{-1})$, where JA^{-1} has rank one since J has rank one. So by Lemma 1.2.5, $\det(J - A) = (-1)^n \det A (1 + \operatorname{tr}(-JA^{-1}))$. Since $A \in S(n, k)$ it follows that $\operatorname{tr}(-JA^{-1}) = -n/k$. Hence

$$\det(J - A) = (-1)^{n-1} \binom{n-k}{k} \det A \quad \square$$

Proposition 1.4.3 establishes a duality between $S(n, k)$ and $S(n, n - k)$. For if $A \in S(n, k)$ and $|\det A| = M(n, k)$, then $J - A \in S(n, n - k)$ and $|\det(J - A)| = \frac{n-k}{k} M(n, k) = M(n, n - k)$ and conversely, since the constants in Proposition 1.4.3 are fixed for any matrix in $S(n, k)$. For $k = 1$, $M(n, 1) = m(n, 1) = 1$, since $S(n, 1) = \{Q : Q \text{ is an } n \times n \text{ permutation matrix}\}$. When $k = n - 1$, using Proposition 1.4.3, it follows that $M(n, n - 1) = n - 1 = m(n, n - 1)$.

We give two examples to illustrate the above ideas.

EXAMPLE 1.4.4 Let $A \in S(6, 3)$. By Theorem 1.2.6, $|\det A| \leq 13.04$. Then by Proposition 1.4.2 it follows that $|\det A| = 9$. Hence $m(6, 3) = M(6, 3) = 9$.

EXAMPLE 1.4.5 Let $A \in S(7, 3)$. Using Theorem 1.2.6 with $k = 3$ and $\lambda = 1$, gives $|\det A| \leq 24$. It is well known that there exists a $(7, 3, 1)$ -configuration that is a projective plane of order 2, hence $M(7, 3) = 24$. A matrix attaining this bound is $I + P + P^3$, where $P = [p_{ij}]$ is the fundamental circulant, i.e. $p_{i, i+1} = 1$ for $i = 1, 2, \dots, n - 1$, $p_{n, 1} = 1$, and $p_{ij} = 0$ otherwise. By Proposition 1.4.3, $M(7, 4) =$

32, and we note that $m(7, 3) = 3$ from Theorem 1.4.1.

For the case $G(n, 1)$, we need only consider $n = 2r$, for some $r \geq 1$. The only regular graph of degree one is a perfect matching, from which it follows that $W(2r, 1) = w(2r, 1) = 1$. The only regular graph of degree $n - 1$ is the complete graph, denoted by K_n , and it follows that $W(n, n - 1) = w(n, n - 1) = n - 1$.

As previously mentioned, Proposition 1.4.3 establishes a duality between $S(n, k)$ and $S(n, n - k)$. Unfortunately, due to the restriction of zero diagonal, the same does not hold for $G(n, k)$. The next result implies a more complicated relationship between $G(n, k)$ and $G(n, n - k - 1)$.

PROPOSITION 1.4.6 *If A is an $n \times n$ $(0, 1)$ matrix with zero trace and constant line sums k , then*

$$\det(J - A - I) = \left(\frac{k + 1 - n}{k + 1} \right) \cdot p_A(-1). \quad (1.2)$$

Proof. If A satisfies the hypotheses, then $I + A$ is in $S(n, k + 1)$ if and only if -1 is not an eigenvalue of A . If -1 is an eigenvalue of A , then the right hand side of (1.2) is zero. Notice that

$$\det(J - A - I) = (-1)^n \cdot p_{J-A}(1).$$

Since A has constant line sums k , A commutes with J , hence the eigenvalues of $J - A$ are $\mu_1 = n - \lambda_1, \mu_i = -\lambda_i$, for $i = 2, 3, \dots, n$, where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A arranged in some order (see [13] Th 2.4.9). Since $J - A$ is an entry-wise nonnegative matrix with Perron root $n - k$, it follows that $\lambda_1 \neq -1$. Thus $\mu_i = 1$ for some $i \geq 2$, hence $\det(J - A - I) = 0$. So (1.2) holds in this case.

If -1 is not an eigenvalue of A , then $I + A \in S(n, k + 1)$, and by Proposition 1.4.3,

$$\det(J - (A + I)) = (-1)^{n-1} \left(\frac{n - (k + 1)}{k + 1} \right) \det(A + I) = \left(\frac{k + 1 - n}{k + 1} \right) p_A(-1)$$

Hence (1.2) holds, and this completes the proof. \square

If $A \in G(n, k)$ and (1.2) is not zero, then $J - A - I \in G(n, n - k - 1)$. We note here that if A is an adjacency matrix of G , then $J - A - I$ is an adjacency matrix of the *complement of G* (see [1] p. 20).

We give two examples to illustrate Proposition 1.4.6.

EXAMPLE 1.4.7 The set $G(6, 3)$ is empty. To prove this, assume to the contrary that there exists $A \in G(6, 3)$, and let $B = J - A - I$. By Proposition 1.4.6, $|\det A| = |\det(J - B - I)| = |p_B(-1)|$. On 6 vertices there are only two graphs (up to isomorphism) regular of degree 2. They are C_6 and $C_3 \cup C_3$, and in either case -1 is an eigenvalue (see [1] p. 17). Hence A is singular, and thus $G(6, 3) = \phi$.

EXAMPLE 1.4.8 Consider $G(10, 3)$ and $G(10, 6)$. Let $A \in G(10, 3)$. Then we need to consider two cases. Suppose $G(A)$ is connected. In [7] Table 3 there is a list of all connected graphs on 10 vertices regular of degree 3. From this table it follows that $W(10, 3) \geq 48$, and $w(10, 3) \leq 3$. By Theorem 1.4.1, $m(10, 3) = 3$, hence $w(10, 3) = 3$. Now suppose $G(A)$ is disconnected. Then, since every component is regular of degree 3, there exist exactly two components of $G(A)$, say G_1, G_2 , with either $|V(G_1)| = 4$ and $|V(G_2)| = 6$ or else $|V(G_1)| = |V(G_2)| = 5$. Since a graph must have an even number of vertices of odd degree, the latter is impossible. Hence G_1 is isomorphic to K_4 . Thus $G(A)$ is isomorphic to $K_4 \cup G_2$ where G_2 is regular of degree 3 with $|V(G_2)| = 6$. From Example 1.4.7 it follows that A is singular, this is a contradiction. Therefore $W(10, 3) = 48$.

If $A \in G(10, 6)$, then $G(B)$ is a regular graph of degree 3, where $B = J - A - I$. If $G(B)$ is connected then we can find $|p_B(-1)|$ in [7] Table 3, otherwise $G(B)$ is disconnected and is isomorphic to $K_4 \cup G_2$ as above. Since -1 is an eigenvalue of $A(K_4)$ this implies $p_B(-1) = 0$. From [7] Table 3 and Proposition 1.4.6, it follows that $w(10, 6) = 12$ and $W(10, 6) = 192$. We remark here that $W(10, 3)$ is attained by the adjacency matrix of the Petersen graph (see [21] p. 10). Also, $W(10, 6)$ is attained by the adjacency matrix of the complement of the Petersen graph.

Chapter 2

Maximum Determinants in $S(n, 2)$ and $G(n, 2)$

In this chapter we begin our study of determining $M(n, k)$ and $W(n, k)$ by considering the case $k = 2$. Our first step is to describe a canonical form for matrices in $S(n, 2)$. We show that every matrix in $S(n, 2)$ is permutationally equivalent to a block diagonal matrix, where each block has the same (0,1) pattern. The sizes of each block may be different. This reduces our study of matrices in $S(n, 2)$ to these block matrices. From our analysis we are able to derive a recurrence relation involving $M(n, 2)$, thus determining $M(n, 2)$.

To determine $W(n, 2)$ and $w(n, 2)$ is easier, since $M(n, 2)$ and $m(n, 2)$ are known and we always have the inequalities:

$$m(n, 2) \leq w(n, 2), \text{ and } W(n, 2) \leq M(n, 2).$$

However, we also derive a canonical form for matrices in $G(n, 2)$. Using the restriction of symmetry and zero trace, we show that every matrix in $G(n, 2)$ is permutationally similar to another block diagonal matrix.

2.1 Maximum Determinants in $S(n, 2)$

When $k = 2$, we stated in the Introduction that $S(n, 2) \neq \phi$ for every n except $n = 4$ (see [16]). We present a proof that shows $S(4, 2) = \phi$. It will become evident that $S(n, 2) \neq \phi$ for $n = 3$ and $n \geq 5$ as we go through this section.

PROPOSITION 2.1.1 $S(4, 2) = \phi$.

Proof. Suppose the contrary, and let $A \in S(4, 2)$. Since there are exactly two ones in row and column 1, we can permute the rows and columns of A so that the resulting matrix has the following form:

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix},$$

where $*$ means either a 0 or 1. Since A is nonsingular, and J_2 is singular, this implies that the (2,2) entry of the above matrix must be zero. Thus by permuting rows and columns 3,4 so that the (2,3) and (3,2) entries are one, this forces the resulting matrix to have the following form

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & * & * \\ 0 & 0 & * & * \end{bmatrix}$$

The (3,3) entry of the above matrix cannot be one since then the (3,4) and (4,3) entries must be zero, but this implies that row 4 does not sum to two. Hence the resulting matrix must be in the form.

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

That is, there exist permutation matrices Q, R such that $QAR = B$. It is straightforward to verify that $\det B = 0$, thus A is singular. This is a contradiction, therefore $S(4, 2) = \phi$. \square

Motivated by the proof above we define the following matrix. For $n \geq 2$, let A_n denote the following $n \times n$ matrix:

$$A_n = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & 0 & 1 \\ 0 & \dots & 0 & 0 & 0 & 1 & 1 \end{bmatrix}. \quad (2.1)$$

LEMMA 2.1.2 For $n \geq 2$,

$$|\det A_n| = \begin{cases} 0 & , \text{ if } n \text{ even,} \\ 2 & , \text{ if } n \text{ odd} \end{cases}$$

Proof. Let R_i denote row i of A_n . Consider the following row operations, $R_2 \leftarrow R_2 - R_1$, $R_3 \leftarrow R_3 + R_2$, and in general for $1 \leq j \leq n-1$, $R_{j+1} \leftarrow R_{j+1} - R_j$ if j is odd and $R_{j+1} \leftarrow R_{j+1} + R_j$ if j is even. Here $R_k \leftarrow R_k + cR_i$ means R_k is replaced with $R_k + cR_i$, which does not alter the value of the determinant. Now if n is even then $n-1$ is odd, and therefore the final row operation is $R_n \leftarrow R_n - R_{n-1}$ leading to a zero row, hence $\det A_n = 0$. If n is odd, then the final row operation is $R_n \leftarrow R_n + R_{n-1}$, giving an upper triangular matrix with main diagonal $(\pm 1, \pm 1, \dots, 2)$, which implies that $|\det A_n| = 2$. \square

Hence when n is odd $A_n \in S(n, 2)$. The following describes a canonical form for matrices in $S(n, 2)$ up to permutation equivalence, see also [4] p. 5. Recall that $B \oplus C$ denotes the direct sum of the matrices B and C , which by definition is

$$B \oplus C = \begin{bmatrix} B & 0 \\ 0 & C \end{bmatrix}.$$

LEMMA 2.1.3 *If $A \in S(n, 2)$, then there exist permutation matrices Q, R such that $QAR = A_{n_1} \oplus A_{n_2} \oplus \dots \oplus A_{n_t}$, with $t \geq 1$, where $\sum_{i=1}^t n_i = n$.*

Proof. The proof is by induction on n . The lemma is readily verified when $n = 3$. Suppose the lemma is true for $A \in S(r, 2)$ where $3 \leq r \leq n-1$. Let $A \in S(n, 2)$. Since there are exactly two nonzero entries in the first row (resp. first column), the rows (resp. columns) of A can be permuted so that $a_{11} = a_{12} = a_{21} = 1$. Thus

$a_{1i} = a_{i1} = 0$ for $i \geq 3$. Since A is nonsingular, $a_{22} = 0$ in which case rows (resp. columns) 3, 4, \dots , n of A can be permuted so that $a_{23} = a_{32} = 1$. Consider two cases. If $a_{33} = 1$, then there exist permutation matrices Q' , R' so that

$$Q'AR' = \begin{bmatrix} A_3 & 0 \\ 0 & A' \end{bmatrix},$$

where $A' \in S(n-3, 2)$, and the result holds by induction. Otherwise $a_{33} = 0$. Then as above, rows (resp. columns) 4, 5, \dots , n of A can be permuted so that $a_{34} = a_{43} = 1$. Now by Lemma 2.1.2, A_4 is singular so it follows that $a_{44} = 0$. Continuing this argument leads to one of two cases. Suppose there exists an odd integer j , $5 \leq j \leq n-2$, with $a_{jj} = 1$. Hence there exist permutation matrices Q'' , R'' so that

$$Q''AR'' = \begin{bmatrix} A_j & 0 \\ 0 & A'' \end{bmatrix},$$

where $A'' \in S(n-j, 2)$, and the result holds by induction. If no such j exists, then either $a_{n-1, n-1} = 1$ or 0. If $a_{n-1, n-1} = 1$, then row n cannot sum to two, so $a_{n-1, n-1} = 0$, hence by the construction $a_{n-1, n} = a_{n, n-1} = 1$, and this forces $a_{nn} = 1$. This completes the proof. \square

As seen in the proof of Lemma 2.1.3, each block matrix A_n has odd order at least 3. For small n , we can now easily construct all matrices in $S(n, 2)$ and thus compute values of $M(n, 2)$. We have already shown that $S(n, n-1) \neq \emptyset$, hence $S(3, 2) \neq \emptyset$. Lemma 2.1.3 implies that if $A \in S(3, 2)$, then there exist permutation

matrices Q, R such that $QAR = A_3$. Since this is true for all $A \in S(3, 2)$, it follows by Lemma 2.1.2 that $M(3, 2) = 2$.

EXAMPLE 2.1.4 We prove that $M(5, 2) = M(7, 2) = 2$, and $M(6, 2) = 4$. Let $A \in S(5, 2)$. Then by Lemma 2.1.3 there exist permutation matrices Q, R such that $QAR = A_5$. Since this is true for all $A \in S(5, 2)$, it follows by Lemma 2.1.2 that $M(5, 2) = 2$. Similar arguments hold for $S(7, 2)$. For $S(6, 2)$, A_6 is singular by Lemma 2.1.2, and there exist permutation matrices Q, R such that $QAR = A_3 \oplus A_3$ by Lemma 2.1.3. Hence $M(6, 2) = 4$, by Lemma 2.1.2.

EXAMPLE 2.1.5 Let $A \in S(9, 2)$. By Lemma 2.1.3, A is permutationally equivalent to either A_9 or $A_3 \oplus A_3 \oplus A_3$. Using Lemma 2.1.2 it follows that $M(9, 2) = 8$, whereas using Theorem 1.4.1, $m(9, 2) = 2$, for $k = 2$ this is the smallest value of n where these extrema are different.

LEMMA 2.1.6 For $n \geq 8$,

$$M(n, 2) = \max \{M(p, 2)M(q, 2) : p, q \geq 3, p + q = n\}. \quad (2.2)$$

Proof. Since for any fixed $r \geq 3$, $r \neq 4$, $S(r, 2)$ is a finite set, there exists $B \in S(r, 2)$ so that $|\det B| = M(r, 2)$. Let $p, q \geq 3$, with $p, q \neq 4$ so that $p + q = n$. Notice

that for $n \geq 8$ we can always find such a p and q . Let $C \in S(p, 2)$, $D \in S(q, 2)$ so that $|\det C| = M(p, 2)$ and $|\det D| = M(q, 2)$. Then $C \oplus D \in S(p + q, 2) = S(n, 2)$ and therefore $M(n, 2) \geq M(p, 2)M(q, 2)$. It follows that

$$M(n, 2) \geq \max \{M(p, 2)M(q, 2) \mid p, q \geq 3, p + q = n\}.$$

Now let $A \in S(n, 2)$. Then by Lemma 2.1.3 there exist permutation matrices Q, R so that $QAR = A_{n_1} \oplus A_{n_2} \oplus \cdots \oplus A_{n_t}$, with $t \geq 1$. If $t > 1$, then since $\det A \neq 0$ it follows that $n_1 \geq 3$ and $n_1 \neq 4$. Thus $QAR = A_{n_1} \oplus B$, where the order of B is also not 4. Then $B \in S(n - n_1, 2)$, and since $|\det A| = |\det A_{n_1}| |\det B|$, this implies

$$|\det A| \leq \max \{M(p, 2)M(q, 2) \mid p, q \geq 3, p + q = n\}.$$

Since $A \in S(n, 2)$ is arbitrary,

$$M(n, 2) \leq \max \{M(p, 2)M(q, 2) \mid p, q \geq 3, p + q = n\}.$$

If $t = 1$, then using Lemma 2.1.2, $|\det A| = 2$ and n must be odd. Since for $n \geq 8$ the right hand side of (2.2) is always greater than 2, the inequality still holds. This completes the proof \square

We come to our main results for the maximum determinant of matrices in $S(n, 2)$

THEOREM 2.1.7 *For $n \geq 8$,*

$$M(n, 2) = 2M(n - 3, 2).$$

Proof. The proof is by induction on n . The cases $n = 8, 9, 10, \dots, 15$ have been verified separately as is necessary because of the restriction on p or q needed in the induction step. Suppose the theorem holds for all s : $15 \leq s \leq n - 1$. Now consider $s = n$. By Lemma 2.1.6,

$$M(n, 2) \geq M(3, 2)M(n - 3, 2) = 2M(n - 3, 2).$$

Also using Lemma 2.1.6, there exist $p, q \geq 3$ and neither equal to 4, so that $p + q = n$ and $M(n, 2) = M(p, 2)M(q, 2)$. Since $n \geq 15$, at least one of p or q is ≥ 8 . Suppose $q \geq 8$. Then by induction

$$M(n, 2) = M(p, 2)M(q, 2) = 2M(p, 2)M(q - 3, 2)$$

Thus by Lemma 2.1.6, $M(n, 2) \leq 2M(n - 3, 2)$. Therefore $M(n, 2) = 2M(n - 3, 2)$

□

COROLLARY 2.1.8 For $n = 3$ and $n \geq 5$,

$$M(n, 2) = \begin{cases} 2^t & , \text{ if } n = 3t \text{ or } n = 3t + 2, \\ 2^{t-1} & , \text{ if } n = 3t + 1. \end{cases}$$

Proof. We use induction on n . Consider the case $n = 3t + 2$. By Theorem 2.1.7 it follows that $M(n, 2) = 2M(n - 3, 2) = 2M(3(t - 1) + 2, 2)$. So by induction

$$M(n, 2) = 2 \cdot 2^{t-1} = 2^t.$$

Similar arguments can be applied when $n = 3t$ and $n = 3t + 1$ \square

COROLLARY 2.1.9 *For $n = 3$ and $n \geq 5$,*

$$M(n, n - 2) = \begin{cases} (n - 2)2^{t-1} & , \text{ if } n = 3t \text{ or } n = 3t + 2, \\ (n - 2)2^{t-2} & , \text{ if } n = 3t + 1. \end{cases}$$

Proof Follows from Proposition 1.4.3 and Corollary 2.1.8. \square

Note that not only do we determine $M(n, 2)$, our proofs also identify matrices attaining $M(n, 2)$. For example, if $n = 3t$, then $A_3 \oplus A_3 \oplus \cdots \oplus A_3$, where there are t copies of A_3 , is in $S(n, 2)$ and has determinant with absolute value 2^t . Similar arguments can be used for $n = 3t + 1, 3t + 2$. Notice that if $n = 3t$, then $|\det(J - (A_3 \oplus A_3 \oplus \cdots \oplus A_3))| = M(n, n - 2)$

By Proposition 1.4.2 if $A \in S(n, k)$, then $|\det A|$ is a multiple of kd , where $d = \gcd(n, k)$. By Lemma 2.1.3 it follows that if $A \in S(n, 2)$, then $|\det A| = 2^r$, for some $r \geq 1$. Thus in the case $k = 2$, the distribution of the values of $|\det A|$ is restricted even more than just being a multiple of $2d$. For example, if $n = 9$, then for $A \in S(9, 2)$, $|\det A| \in \{2, 2^3\}$, so $|\det A| \neq 4$ or 6 . For general n , write $n = \sum_{i=1}^r n_i$, where $r \geq 1$, $n_i \geq 3$ and odd. Then for $A \in S(n, 2)$, $|\det A| = 2^r$, and every such value can be achieved. For $k = 2$, this answers a question posed by Grady and Newman in [10] concerning the distribution of the values of $|\det A|$ when

$A \in S(n, k)$.

2.2 Maximum Determinants in $G(n, 2)$

Now we consider the set $G(n, 2)$, and begin with some graph theoretic results, the first of which can be found in [21] p. 11. Recall that C_n is an n -cycle, as defined in Chapter 1.

LEMMA 2.2.1 *Let $G = (V, E)$ be a connected graph on n vertices that is regular of degree 2. Then G is isomorphic to C_n .*

Proof. Since G is connected and $|V| = |E|$ it follows that G contains a cycle (see [21]). Since any vertex in this cycle has degree two, any vertex in the cycle cannot be connected to any vertex not in the cycle. However, G is connected, hence the cycle must include every vertex, that is G is isomorphic to C_n . \square

COROLLARY 2.2.2 *If $G = (V, E)$ is a regular graph of degree 2, then G is a union of cycles.*

The adjacency matrix of C_n is written out below as it will be useful later.

$$A(C_n) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & \dots & 1 \\ 1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & 0 & 1 \\ 1 & \dots & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad (2.3)$$

The following is a well known result and can be found in [7] p 306

LEMMA 2.2.3 *If $A(C_n)$ is an $n \times n$ adjacency matrix of C_n , then*

$$|\det A(C_n)| = \begin{cases} 0 & , \text{ if } n \equiv 0 \pmod{4}, \\ 2 & , \text{ if } n \equiv 1 \text{ or } 3 \pmod{4}, \\ 4 & , \text{ if } n \equiv 2 \pmod{4} \end{cases}$$

If $A \in G(n, 2)$, then Corollary 2.2.2 characterizes $G(A)$. Knowing this fact and using Lemma 2.2.3, we determine $W(n, 2)$ and $w(n, 2)$.

THEOREM 2.2.4 *For $n = 3$ and $n \geq 5$,*

$$W(n, 2) = M(n, 2) \text{ and } w(n, 2) = m(n, 2),$$

where $M(n, 2)$ is given by Corollary 2.1.8 and $m(n, 2)$ by Theorem 1.4.1

Proof. The case $n = 3$ has already been done in Section 1.4. So suppose $n \geq 5$. First, let $n = 3t$ for some $t \geq 2$. Let $B = A(C_3) \oplus A(C_3) \oplus \dots \oplus A(C_3)$

be the direct sum of t copies of $A(C_3)$. Then $B \in G(n, 2)$ and by Lemma 2 2 3, $|\det B| = 2^t$. Hence by Corollary 2 1 8

$$W(n, 2) \geq |\det B| = 2^t = M(n, 2) \geq W(n, 2),$$

since $G(n, 2) \subset S(n, 2)$. For the case $n = 3t + 1$, let

$B = A(C_3) \oplus A(C_3) \oplus \cdots \oplus A(C_3) \oplus A(C_7)$, where there are $t - 2$ copies of $A(C_3)$

and apply similar arguments as above. Similarly if $n = 3t + 2$, let

$B = A(C_3) \oplus A(C_3) \oplus \cdots \oplus A(C_3) \oplus A(C_5)$ with $t - 1$ copies of $A(C_3)$.

For the minimum, similar arguments can be applied depending on whether n is even or odd. For example, if n is odd, then $m(n, 2) = 2$, and if we let $B = A(C_n)$, then $B \in G(n, 2)$ and by Lemma 2 2 3

$$w(n, 2) \leq |\det B| = 2 = m(n, 2) \leq w(n, 2)$$

Hence $w(n, 2) = m(n, 2)$. \square

Chapter 3

Maximum Determinants in $G(n, n - 3)$ and $S(n, n - 3)$

In this chapter we begin our analysis by considering $G(n, n - 3)$. We determine $W(n, n - 3)$ and $w(n, n - 3)$, for $n = 4, 5$ and $n \geq 7$. Knowing $W(n, n - 3)$ gives rise to new lower bounds for $M(n, n - 3)$ and $M(n, 3)$.

3.1 Preliminaries

If $A \in G(n, n - 3)$, then let $B = J - A - I$. Using Corollary 2.2.2 we know that $G(B)$ is a union of cycles. By Proposition 1.4.6,

$$|\det A| = |\det(J - B - I)| = \left(\frac{n-3}{3}\right) \cdot |p_B(-1)|.$$

So in order to maximize $|\det A|$ we need to maximize $|p_B(-1)|$. However, first we need to understand more about $p_{A(C_n)}(-1)$ since $G(B)$ is a union of cycles. As in Example 1.4.5, we denote the fundamental circulant by P . It is readily verified that the characteristic polynomial of P is $\lambda^n - 1$. Hence the eigenvalues of P are the n th roots of unity, $\omega_j = \cos\left(\frac{2\pi j}{n}\right) + i \sin\left(\frac{2\pi j}{n}\right)$, $0 \leq j \leq n - 1$. Referring to (2.3) gives $A(C_n) = P + P^{-1}$, note that $P^{-1} = P^{n-1}$. If f is any polynomial, then $f(\lambda)$

is an eigenvalue of $f(A)$, where λ is an eigenvalue of A . Thus the eigenvalues of $A(C_n)$ are $\omega_j + \omega_j^{-1}$, $0 \leq j \leq n-1$. Since ω_j is on the unit circle, its inverse is equal to its complex conjugate. Hence the eigenvalues of $A(C_n)$ are $2 \cos(\frac{2\pi j}{n})$, for $j = 0, 1, \dots, n-1$ (see also [7] p. 306). Therefore -1 is an eigenvalue of $A(C_n)$ if and only if there exists j such that $\cos(\frac{2\pi j}{n}) = -1/2$. This implies that either $\frac{2\pi j}{n} = \frac{2\pi}{3}$ or $\frac{2\pi j}{n} = \frac{4\pi}{3}$. In either case we have that $n = 3t$, for some positive integer t . Therefore $p_{A(C_n)}(-1) = 0$ if and only if $n = 3t$, for $t \geq 1$. We give an example for illustration.

EXAMPLE 3.1.1 We claim that up to permutation similarity there is only one matrix in $G(7, 4)$. Let $A \in G(7, 4)$ and $B = J - A - I$. There are essentially only two graphs on 7 vertices regular of degree 2, namely C_7 and $C_3 \cup C_4$. If B is the adjacency matrix of $C_3 \cup C_4$, then from the remarks above -1 is an eigenvalue of B (see also [1] p. 17). However, if B is the adjacency matrix of C_7 , then -1 is not an eigenvalue of B , and $|p_B(-1)| = 3$ (see [7] p. 306). Hence, $w(7, 4) = W(7, 4) = 4$ by Proposition 1.4.6.

Recall that we have already shown that $G(6, 3) = \phi$ (see Example 1.4.7), and we will show that $G(n, n-3) \neq \phi$ for $n = 4, 5$ and $n \geq 7$. Compare this with the fact that $S(4, 2) = \phi$, and $S(n, 2) \neq \phi$ for $n = 3$ and $n \geq 5$.

3.2 Maximum Determinants in $G(n, n-3)$

LEMMA 3.2.1 For $n \geq 3$,

$$p_{A(C_n)}(-1) = \begin{cases} 0 & , \text{ if } n = 3t, \\ -3 & , \text{ otherwise} \end{cases}$$

Proof. When $n = 3t$, we have already shown in Section 3.1 that $p_{A(C_n)}(-1) = 0$.

For $n \geq 3$, we claim that the following holds,

$$p_{A(C_{n+3})}(-1) = p_{A(C_n)}(-1)$$

To prove this claim, notice that

$$p_{A(C_{n+3})}(-1) = \det \begin{bmatrix} -1 & -1 & 0 & 0 & 0 & \dots & -1 \\ -1 & -1 & -1 & 0 & 0 & \dots & 0 \\ 0 & -1 & -1 & -1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & -1 & -1 & -1 & 0 \\ 0 & \dots & 0 & 0 & -1 & -1 & -1 \\ -1 & \dots & 0 & 0 & 0 & -1 & -1 \end{bmatrix},$$

hence,

$$p_{A(C_{n+3})}(-1) = (-1)^{n+3} \det \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & \dots & 1 \\ 1 & 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \dots & 0 & 1 & 1 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 & 1 & 1 \\ 1 & \dots & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \quad (3.1)$$

Thus

$$p_{A(C_{n+3})}(-1) = (-1)^{n+3} \det(L_{n+3}),$$

where L_{n+3} is defined as the matrix in (3.1) above.

We use elementary row operations to compute the determinant of L_{n+3} . Perform the following row operations $R_2 \leftarrow R_2 - R_1$ and $R_{n+3} \leftarrow R_{n+3} - R_1$. Then

$$\det(L_{n+3}) = \det \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & \cdots & 1 \\ 0 & 0 & 1 & 0 & 0 & \cdots & -1 \\ 0 & 1 & 1 & 1 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \vdots & \cdots & 1 & 1 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 1 & 1 \\ 0 & -1 & \cdots & 0 & 0 & 1 & 0 \end{bmatrix}. \quad (3.2)$$

Now replace R_{n+2} by $R_{n+2} + R_2$, and replace R_3 by $R_3 + R_{n+3}$. This does not alter the value of the determinant of (3.2) and gives

$$\det(L_{n+3}) = \det \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & -1 \\ 0 & 0 & 1 & 1 & 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \ddots & \ddots & \ddots & & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 \end{bmatrix}. \quad (3.3)$$

Expand this determinant by the first column, and then expand the resulting determinant by the first column. The final step is to expand the resulting determinant

by the last column, giving

$$\det(L_{n+3}) = (-1)^{2(n+3)+1} \det \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 1 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 1 & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & 0 & 1 & 1 & 1 & 0 \\ 0 & \cdots & 0 & 0 & 1 & 1 & 1 \\ 1 & \cdots & 0 & 0 & 0 & 1 & 1 \end{bmatrix}, \quad (3.4)$$

where the above matrix is $n \times n$. Hence (3.4) implies that

$$\det(L_{n+3}) = (-1)^{2(n+3)+1} \det(L_n)$$

Thus combining this and (3.1), it follows that

$$p_{A(C_{n+3})}(-1) = (-1)^{n+3} (-1)^{2(n+3)+1} (-1)^n p_{A(C_n)}(-1) = p_{A(C_n)}(-1).$$

This proves the claim. It is readily verified that $p_{A(C_3)}(-1) = 0$, and

$p_{A(C_4)}(-1) = p_{A(C_5)}(-1) = -3$, thus the result follows by a simple induction argument. \square

THEOREM 3.2.2 For $n = 4, 5$ and $n \geq 7$,

$$w(n, n-3) = m(n, n-3) = \begin{cases} 3(n-3) & , \text{ if } n = 3t, \\ (n-3) & , \text{ otherwise} \end{cases}$$

Proof. The result for $m(n, n-3)$ follows from Theorem 1.4.1. For $w(n, n-3)$, suppose $n \neq 3t$. If $B = A(C_n)$ it follows that $J - B - I \in G(n, n-3)$, since

$J - B - I$ is nonsingular by Lemma 3.2.1. Using Proposition 1.4.6 and Lemma 3.2.1 again,

$$|\det(J - B - I)| = \binom{n-3}{3} \cdot |p_B(-1)| = n - 3.$$

If $n = 3t$, then write $n = 4 + 3(t - 2) + 2$. Let $B = A(C_4) \oplus A(C_{3(t-2)+2})$. Using similar arguments as above, it follows that $|\det(J - B - I)| = 3(n - 3)$. \square

In order to determine $W(n, n - 3)$ it is convenient to let

$$\mu_n = \max\{|p_B(-1)| : B \text{ is an } n \times n \text{ adjacency matrix of a regular graph of degree } 2\}.$$

By the remarks in Section 3.1, for $n = 4, 5$ and $n \geq 7$,

$$W(n, n - 3) = \binom{n-3}{3} \mu_n. \quad (3.5)$$

The proof of the following lemma is similar to the proof of Lemma 2.1.6 and is omitted.

LEMMA 3.2.3 For $n \geq 8$,

$$\mu_n = \max\{\mu_p \cdot \mu_q : p, q \geq 3, p + q = n\}.$$

Evaluation of μ_n leads to our main results for the maximum absolute value of the determinant of matrices in $G(n, n - 3)$.

THEOREM 3.2.4 For $n \geq 11$,

$$\mu_n = 3\mu_{n-4}$$

Proof The proof is by induction on n . The cases $n = 11, 12, \dots, 21$, have been verified separately as is necessary for the induction step. So suppose the result is true for s , where $21 \leq s \leq n-1$. Now consider $s = n$. By Lemma 3.2.3,

$$\mu_n \geq \mu_4 \cdot \mu_{n-4} = 3 \cdot \mu_{n-4}$$

However, by Lemma 3.2.3 there exist $p, q \geq 3, p+q = n$, such that $\mu_n = \mu_p \cdot \mu_q$, and we may assume without loss of generality that $q \geq 11$. Therefore by induction $\mu_q = 3 \cdot \mu_{q-4}$. Using Lemma 3.2.3, it follows that $\mu_n \leq 3 \cdot \mu_{n-4}$. \square

For $x \in \mathbf{R}$, let $[x]$ denote the largest integer smaller than or equal to x . The following can be proved easily by verifying the smaller cases separately, and using induction for $n \geq 11$.

COROLLARY 3.2.5 For $n = 4, 5$ and $n \geq 7$, $\mu_n = 3^{\lfloor n/4 \rfloor}$

Combining Corollary 3.2.5 and (3.5), gives the following

THEOREM 3.2.6 For $n = 4, 5$ and $n \geq 7$,

$$W(n, n-3) = (n-3)3^{\lfloor n/4 \rfloor - 1}$$

Since $G(n, n-3) \subset S(n, n-3)$, and using the duality in Proposition 1.4.3, Theorem 3.2.6 gives the following new bounds for $M(n, n-3)$ and $M(n, 3)$.

COROLLARY 3.2.7 For $n = 4, 5$ and $n \geq 7$,

$$M(n, n-3) \geq (n-3)3^{\lfloor n/4 \rfloor - 1}, \text{ and } M(n, 3) \geq 3^{\lfloor n/4 \rfloor}.$$

Note that in general the bounds given in Corollary 3.2.7 are not tight. In particular, for $n = 10$, it was shown in Example 1.4.8 that $W(10, 3) = 48$. This implies that $M(10, 3) \geq 48$. However, the bound given in Corollary 3.2.7 gives $M(10, 3) \geq 9$. Combining Corollary 3.2.7 and Theorem 1.2.6 implies

$$3^{\lfloor n/4 \rfloor} \leq M(n, 3) \leq 3^{\frac{n+1}{2}}.$$

Chapter 4

Related Applications

In this final chapter, we present some independent but related results concerning $S(n, k)$ and $G(n, k)$. Specifically, we show that there exist permutation matrices Q, R such that $QA_nR = A(C_n)$ if and only if n is odd. We also establish another relationship between A_n and $A(C_n)$ that leads to a method for computing the eigenvalues of the class of tridiagonal matrices $aI_n + bA_n$, where $a, b \in \mathbf{R}$.

As a final topic we use a result of [8] to give a localization result for the subdominant eigenvalues of symmetric $(0,1)$ matrices with constant line sums and zero trace. We then establish a better localization result for the subdominant eigenvalues of the matrices above, and show that in general this region cannot be improved. We conclude the chapter with a brief summary of the results contained in the thesis and present a table of presently known values of $m(n, k)$, $w(n, k)$, $W(n, k)$ and $M(n, k)$.

4.1 Relationship between $S(n, 2)$ and $G(n, 2)$

In this section we provide a relationship between A_n and $A(C_n)$. We already

know that since $A(C_n) \in S(n, 2)$ there exist permutation matrices Q, R such that $QA(C_n)R$ is equal to a direct sum of matrices of the form A_n . However, we will prove that more is true. First we need some definitions and basic facts for (0,1) matrices, see [4] Chap. 3 and 4 for more details

DEFINITION 4.1.1 If A is an $n \times n$ (0,1) matrix with $n \geq 2$, then A is *partly decomposable* if there exist permutation matrices Q, R such that

$$QAR = \begin{bmatrix} B & 0 \\ C & D \end{bmatrix},$$

where 0 is a $t \times (n - t)$ matrix, $1 \leq t \leq n - 1$, and B, D are square matrices. Otherwise A is *fully indecomposable*. A is said to be *nearly decomposable* if A is fully indecomposable, and if any 1 is replaced by a zero the resulting matrix is partly decomposable. A is *reducible* if there exists a permutation matrix Q such that

$$QAQ^T = \begin{bmatrix} B & 0 \\ C & D \end{bmatrix},$$

where 0 is a $t \times (n - t)$ matrix, $1 \leq t \leq n - 1$, and B, D are square matrices. Otherwise A is *irreducible*.

If A is an $n \times n$ symmetric (0,1) matrix with zero trace and A is irreducible, then it follows that $G(A)$ is connected (see [2] p. 30).

The case when $n = 1$ is either trivial or non instructive, so we assume henceforth that $n \geq 2$. The following lemma can be found in [4] p. 113.

LEMMA 4.1.2 *If A is an $n \times n$ $(0,1)$ matrix, then A is fully indecomposable if and only if there exist permutation matrices Q, R such that QAR is irreducible, with each diagonal entry equal to 1*

COROLLARY 4.1.3 *If A is an $n \times n$ $(0,1)$ fully indecomposable matrix, then A contains at least $2n$ ones.*

Proof. This result follows directly from the definition of irreducibility and Lemma 4.1.2. \square

PROPOSITION 4.1.4 *A_n is fully indecomposable.*

Proof. Let C_i denote the i th column of A_n in (2.1). Consider two cases. If n is odd, then for $i = 1, 2, \dots, \lfloor n/2 \rfloor$, interchange C_{2i} and C_{2i+1} . The resulting matrix has each diagonal entry equal to 1. Thus there exist permutation matrices Q', R' ($Q' = I$) such that $Q'AR' = I + H$, where H is a permutation matrix given by the permutation $(1, 3, 5, \dots, n, n-1, n-3, \dots, 2)$. Hence H is an irreducible matrix, and therefore $Q'AR'$ is an irreducible matrix. By Lemma 4.1.2, A_n is fully indecomposable. For the case when n is even, let $i = 1, 2, \dots, \lfloor n/2 \rfloor - 1$ and apply similar arguments. \square

PROPOSITION 4.1.5 *A_n is nearly decomposable.*

Proof By Proposition 4.1.4, A_n is fully indecomposable. Moreover since A_n has exactly $2n$ ones, A_n is nearly decomposable by Corollary 4.1.3. \square

PROPOSITION 4.1.6 $A(C_n)$ is nearly decomposable if and only if n is odd.

Proof. Suppose n is odd. Recall from (2.3) that $A(C_n) = P + P^{-1}$, where P is the fundamental circulant. Since n is odd, P^2 is an irreducible matrix. Thus since $PA(C_n)I = I + P^2$, by Lemma 4.1.2 $A(C_n)$ is fully indecomposable. Using similar arguments as in Proposition 4.1.5, it follows that $A(C_n)$ is nearly decomposable. To prove the converse, suppose n is even. To show $A(C_n)$ is not nearly decomposable it is sufficient to show that $A(C_n)$ is partly decomposable. Let $n = 2s$, for some $s \geq 1$, also let $X = \{2, 4, \dots, 2s\}$, and $Y = \{1, 3, \dots, 2s - 1\}$. Permute the rows of $A(C_n)$ so that all the indices corresponding to Y are before the indices corresponding to X , and permute the columns of $A(C_n)$ so that all the indices corresponding to X are before the indices corresponding to Y . Thus there exist permutation matrices Q, R so that

$$QA(C_n)R = \begin{bmatrix} A' & 0 \\ 0 & A'' \end{bmatrix},$$

where 0 is $s \times s$. Hence $A(C_n)$ is partly decomposable when n is even. \square

The following can be found in [4] p. 122.

LEMMA 4.1.7 Suppose A is an $n \times n$ $(0,1)$ matrix. If A is nearly decomposable

and the total number of ones in A is $2n$, then there exist permutation matrices Q, R such that $QAR = I + P$.

THEOREM 4.1.8 *There exist permutation matrices Q, R such that $QA_nR = A(C_n)$ if and only if n is odd*

Proof. Suppose n is odd. By Propositions 4.1.5 and 4.1.6, both A_n and $A(C_n)$ are nearly decomposable. Thus by Lemma 4.1.7, it follows that there exist permutation matrices Q', R', Q'', R'' such that

$$Q'A_nR' = I + P = Q''A(C_n)R''$$

Hence there exist permutation matrices Q, R such that $QA_nR = A(C_n)$. To prove the converse, suppose there exist permutation matrices Q, R such that $QA_nR = A(C_n)$. Since A_n is fully indecomposable by Proposition 4.1.4, it follows from Definition 4.1.1 that $A(C_n)$ is fully indecomposable. Hence n is odd by Proposition 4.1.6. \square

Note that Theorem 4.1.8 gives another proof of Theorem 2.2.4 in the case n odd.

4.2 Eigenvalues of a Class of Tridiagonal Matrices

In this section we derive a formula for the eigenvalues of the class of matrices in

the following form

$$aI_n + bA_n = \begin{bmatrix} (a+b) & b & 0 & 0 & 0 & \dots & 0 \\ b & a & b & 0 & 0 & \dots & 0 \\ 0 & b & a & b & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \dots & 0 & b & a & b & 0 \\ 0 & \dots & 0 & 0 & b & a & b \\ 0 & \dots & 0 & 0 & 0 & b & (a+b) \end{bmatrix}, \quad (4.1)$$

where $a, b \in \mathbf{R}$

If λ is an eigenvalue of A , then λ^2 is an eigenvalue of A^2 , since if $Ax = \lambda x$, then

$$A^2x = A(Ax) = \lambda Ax = \lambda^2x.$$

Moreover a partial converse is true, that is if λ is an eigenvalue of A^2 , then there exists β an eigenvalue of A such that $\beta^2 = \lambda$. As there are only n eigenvalues, this implies that either $\beta = \sqrt{\lambda}$ or $\beta = -\sqrt{\lambda}$. We use this fact later.

The following is a well known result on the eigenvalues of a tridiagonal matrix (see [17], [12]), although we present a different proof here for completeness.

LEMMA 4.2.1 *Let T be an $n \times n$ matrix in the following form*

$$T = \begin{bmatrix} a_1 & b_1 & 0 & 0 & 0 & \dots & 0 \\ c_1 & a_2 & b_2 & 0 & 0 & \dots & 0 \\ 0 & c_2 & a_3 & b_3 & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \dots & 0 & c_{n-3} & a_{n-2} & b_{n-2} & 0 \\ 0 & \dots & 0 & 0 & c_{n-2} & a_{n-1} & b_{n-1} \\ 0 & \dots & 0 & 0 & 0 & c_{n-1} & a_n \end{bmatrix}. \quad (4.2)$$

If $b_i c_i > 0$, for $i = 1, 2, \dots, n-1$, then the eigenvalues of T are real and have algebraic multiplicity one (i.e. are simple).

Proof. Let $D = [d_{ij}]$ be the $n \times n$ diagonal matrix where $d_{11} = 1$, and for $k > 1$, $d_{kk} = \sqrt{\frac{b_1 b_2 \dots b_{k-1}}{c_1 c_2 \dots c_{k-1}}}$. Then it is readily verified that

$$DTD^{-1} = \begin{bmatrix} a_1 & \sqrt{b_1 c_1} & 0 & 0 & 0 & \dots & 0 \\ \sqrt{b_1 c_1} & a_2 & \sqrt{b_2 c_2} & 0 & 0 & \dots & 0 \\ 0 & \sqrt{b_2 c_2} & a_3 & \sqrt{b_3 c_3} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & \sqrt{b_{n-3} c_{n-3}} & a_{n-2} & \sqrt{b_{n-2} c_{n-2}} & 0 \\ 0 & \dots & 0 & 0 & \sqrt{b_{n-2} c_{n-2}} & a_{n-1} & \sqrt{b_{n-1} c_{n-1}} \\ 0 & \dots & 0 & 0 & 0 & \sqrt{b_{n-1} c_{n-1}} & a_n \end{bmatrix}$$

Since DTD^{-1} is symmetric and T and DTD^{-1} have the same eigenvalues, this implies that the eigenvalues of T are real. Moreover this relation implies that the algebraic multiplicity (i.e. the multiplicity of the zero in the characteristic polynomial) equals the geometric multiplicity (i.e. the dimension of the eigenspace) for each eigenvalue of T (see [13] p. 103). Suppose λ is an eigenvalue of T . Then $\lambda I - T$ is also of the form (4.2). If the first row and last column of $\lambda I - T$ is deleted, then the resulting matrix is an $(n-1) \times (n-1)$ upper triangular matrix with no zero entries on the diagonal since $b_i c_i > 0$, for $i = 1, 2, \dots, n-1$. Hence this submatrix has rank $n-1$. So, it follows that $\lambda I - T$ has rank at least $n-1$ (see [13] p. 13). However, $\lambda I - T$ has rank at most $n-1$ since λ is an eigenvalue of T . So by definition λ has geometric multiplicity one. This completes the proof. \square

The following proposition gives rise to another relationship between A_n and $A(C_n)$.

PROPOSITION 4.2.2 *If $n \geq 3$, then $A_n A_n^T - 2I = A_n^2 - 2I$ is permutationally similar to $A(C_n)$. In particular, if n is odd, then $A_n^2 - 2I \in G(n, 2)$.*

Proof. It is an easy computation to verify that

$$A_n^2 - 2I = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & \cdots & 1 & 0 & 0 & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 1 & 0 \end{bmatrix}$$

The first assertion can be verified by considering $G(A_n^2 - 2I)$ and checking that this graph is isomorphic to C_n . For n odd, $A(C_n)$ is nonsingular by Lemma 2.2.3, giving the second assertion. \square

Proposition 4.2.2 gives as a corollary, a simple method of computing the eigenvalues of A_n , see [11] for a statement of this result

COROLLARY 4.2.3 *For $n \geq 2$, the eigenvalues of A_n are*

$$\lambda_j = 2 \cos\left(\frac{\pi j}{n}\right), \quad \text{for } 0 \leq j \leq n-1.$$

Proof. For the case $n = 2$, note that $A_2 = J_2$ and since the eigenvalues of J_2 are 0 and 2 the result holds. Suppose $n \geq 3$. Then by Proposition 4.2.2 the eigenvalues of $A_n^2 - 2I$ are equal to the eigenvalues of $A(C_n)$. The eigenvalues of $A(C_n)$ are $2 \cos(\frac{2\pi j}{n})$ for $j = 0, 1, \dots, n-1$, see Section 3.1. If λ^2 is an eigenvalue of A_n^2 , then

$$\lambda^2 = 2 \cos\left(\frac{2\pi j}{n}\right) + 2 = 4 \cos^2\left(\frac{\pi j}{n}\right),$$

for some j , $0 \leq j \leq n-1$. Thus $\lambda = \pm 2 \cos(\frac{\pi j}{n})$, and either λ or $-\lambda$ is an eigenvalue of A_n . For each j , $0 \leq j \leq n-1$, let $\lambda_j = 2 \cos(\frac{\pi j}{n})$. Then

$$-\lambda_j = 2 \cos\left(\pi - \frac{\pi j}{n}\right) = 2 \cos\left(\frac{\pi(n-j)}{n}\right) = \lambda_{n-j}$$

Thus for $j \geq 1$ either λ_j or λ_{n-j} is an eigenvalue of A_n . Since A_n is a tridiagonal matrix with positive super and subdiagonals, the eigenvalues of A_n are simple by Lemma 4.2.1. Hence for $j \geq 1$, λ_j is an eigenvalue of A_n . For the case when $j = 0$, it is easy to see that 2 is an eigenvalue of A_n , and this completes the proof. \square

THEOREM 4.2.4 For $n \geq 2$, the eigenvalues of the matrix given by (4.1), namely $aI_n + bA_n$, are

$$\lambda_j = a + 2b \cos\left(\frac{\pi j}{n}\right), \quad \text{for } j = 0, 1, \dots, n-1.$$

Proof. Follows from Corollary 4.2.3.

4.3 On the Eigenvalues of Matrices in $G(n, k)$

In this section we give a new localization result on the eigenvalues of symmetric $(0,1)$ matrices with constant line sums and zero trace, and in particular the matrices in $G(n, k)$. One localization result is a direct consequence of the Perron-Frobenius theorem (Theorem 1.2.1), which gives that if $A \in G(n, k)$, then any eigenvalue λ of A satisfies $|\lambda| \leq k$, and $\lambda \in \mathbf{R}$. However, Theorem 1.2.1 is satisfied by any entry-wise nonnegative matrix, and matrices in $G(n, k)$ have a lot more structure, namely, they have constant line sums and are symmetric $(0,1)$ matrices with zero trace.

We state a result that was proved in [8]. The authors of [8] were concerned with the location of eigenvalues of real matrices B that satisfied $Be = \rho(B)e$, sometimes called *stochastic* matrices. Smith [20] also used this result to describe the location of the eigenvalues of a special class of matrices known as *Z*-matrices. We also assume that $n \geq 2$. We say that λ is a *subdominant eigenvalue* of A if $|\lambda| < \rho(A)$.

THEOREM 4.3.1 (Deutsch-Zenger) *If $B = [b_{ij}]$ is an $n \times n$ real matrix with $Be = \rho(B)e$, then all the eigenvalues other than $\rho(B)$ lie in*

$$\Pi(B) = \cup_{i \neq j} \Pi_{ij}(B),$$

where

$$\begin{aligned}\Pi_{ij}(B) &= \{m_{ij} + ur_{ij} + zh_{ij} : z \in Z', |u| \leq 1\}, \\ m_{ij} &= (b_{ii} + b_{jj} - b_{ij} - b_{ji})/2, \quad h_{ij} = |b_{ii} - b_{jj} + b_{ij} - b_{ji}|, \\ d_{ij} &= \frac{1}{2} \sum_{l \neq i, j} |b_{il} - b_{jl}|, \quad r_{ij} = d_{ij} - h_{ij}/2 \quad \text{and} \\ Z' &= \{z : |z - 1/2| \leq 1, |z + 1/2| \leq 1\}.\end{aligned}$$

PROPOSITION 4.3.2 *Let A be an $n \times n$ symmetric $(0,1)$ matrix with zero trace and constant line sums k . Then for each $1 \leq i, j \leq n$,*

$h_{ij} = 0$, $m_{ij} = -a_{ij}$ and

$$r_{ij} = d_{ij} = \frac{1}{2} \left(\sum_{l=1}^n |a_{il} - a_{jl}| \right) - a_{ij},$$

where h_{ij} , m_{ij} , r_{ij} , and d_{ij} are defined in Theorem 4.3.1. Moreover, if $A \in G(n, k)$,

then

$$-1/2 \leq r_{ij} \leq \begin{cases} k & , \text{ if } k \leq n/2, \\ n - k & , \text{ if } k > n/2 \end{cases}$$

Proof. Using the fact that A is a symmetric $(0,1)$ matrix with zero trace, the results for m_{ij} and h_{ij} follow immediately from the definitions in Theorem 4.3.1.

Since $h_{ij} = 0$, this implies that $r_{ij} = d_{ij}$. For r_{ij} consider the following,

$$r_{ij} = \frac{1}{2} \sum_{l \neq i, j} |a_{il} - a_{jl}| = \frac{1}{2} \left(\sum_{l=1}^n |a_{il} - a_{jl}| - 2a_{ij} \right),$$

since $a_{ii} = 0$ for all i . Hence the first result for r_{ij} follows.

To prove the second assertion notice that the quantity in the brackets represents the differences in the row sums of rows i, j of A . Let R_i, R_j denote rows i, j of A , respectively. For the lower bound on r_{ij} , if $\sum_l |a_{il} - a_{jl}| = 0$, then $R_i = R_j$ which implies that A is singular. Thus since $A \in G(n, k)$, $\sum_l |a_{il} - a_{jl}| > 0$. Since A is also a $(0,1)$ matrix we must have $\sum_l |a_{il} - a_{jl}| \geq 1$, hence $r_{ij} \geq -1/2$. For the upper bound, we note that the sum $\sum_l |a_{il} - a_{jl}|$ is invariant under any column permutation, hence we can assume that $R_i = (1, 1, \dots, 1, 0, 0, \dots, 0)$, where there are k consecutive ones followed by $n - k$ consecutive zeros in R_i . Now it is straightforward to verify that

$$\sum_{l=1}^n |a_{il} - a_{jl}| \leq \begin{cases} 2k & , \text{ if } k \leq n/2 \\ 2(n - k) & , \text{ if } k > n/2 \end{cases}$$

Since $a_{ij} = 0$ or 1 the bounds for r_{ij} follows. \square

By Proposition 4.3.2 it follows that

$$\Pi_{ij}(A) = \{m_{ij} + ur_{ij} : |u| \leq 1\}$$

Thus for each $1 \leq i, j \leq n$, $\Pi_{ij}(A)$ is a disc in the complex plane centered at m_{ij} of radius r_{ij} . Note that for $A \in G(n, k)$, $m_{ij} = -1$ or 0 .

First we consider the case when $k \leq n/2$. Then $r_{ij} \leq k$ by Proposition 4.3.2

Thus all we can conclude about the subdominant eigenvalues of $A \in G(n, k)$ is

that they lie in the set $\{z : |z| \leq k\}$, which is exactly equal to the disc given by the Perron-Frobenius theorem (Theorem 1.2.1). One of the reasons that Theorem 4.3.1 is not very useful is the fact that when $A \in G(n, k)$, with $k \leq n/2$, then A may be reducible. Hence $\rho(A)$ may not be a simple eigenvalue (see [13] p. 508). Thus we expect the discs for the remaining eigenvalues to include the disc given by Theorem 1.2.1.

Consider the case when $k > n/2$. If $A \in G(n, k)$, with $k > n/2$, then it is easy to see that $G(A)$ is connected. Hence A is irreducible. Therefore $\rho(A)$ is a simple eigenvalue of A (see [13] p. 508). Thus the discs given by Theorem 4.3.1 give a better estimate on the location of the other eigenvalues of A .

THEOREM 4.3.3 *Let A be an $n \times n$ symmetric $(0,1)$ matrix with zero trace and constant line sums k . If $k > n/2$ and $\lambda \neq k$ is any eigenvalue of A , then*

$$|\lambda| \leq (n - k) + 1.$$

Proof. If $k > n/2$, then $r_{ij} \leq n - k$ by Proposition 4.3.2. This implies that $\Pi_{ij}(A)$ is centered at 0 or -1 and has a maximum possible radius $n - k$. Thus the maximum absolute value of λ is $(n - k) + 1$. \square

We remark here that Theorem 4.3.3 holds for any matrix in $G(n, k)$. By Theorem

4 3 3, if $A \in G(n, n - 3)$, then any eigenvalue $\lambda \neq n - 3$ of A satisfies $|\lambda| \leq 4$. However, we now show that this bound is never attained, and obtain a sharper bound, that in general cannot be improved.

THEOREM 4.3.4 *Let A be an $n \times n$ symmetric $(0, 1)$ matrix with zero trace and constant line sums k . If $k > n/2$ and $\lambda \neq k$ is any eigenvalue of A , then*

$$|\lambda| \leq n - k$$

Equality holds for some $\lambda \neq k$ if and only if $J - A - I$ is reducible.

Proof. For simplicity of notation let $B = J - A - I$. Then B satisfies the same hypotheses as A except that B has constant line sums $n - k - 1$. Since J and $B + I$ commute it follows that the eigenvalues of $A = J - (B + I)$ are $\lambda_1 = n - \mu_1 - 1$ and $\lambda_i = -\mu_i - 1$, $i \geq 2$, where $\mu_1, \mu_2, \dots, \mu_n$ are the eigenvalues of B arranged in some order. We claim that $\lambda_1 = \rho(A) = k$. To prove this, suppose not, that is, suppose there exists λ_i with $i \geq 2$, such that $\lambda_i = k$. Since $k > n/2$, A is irreducible, and this λ_i must be unique. Therefore $-\mu_i = k + 1$, implying that $|\mu_i| = k + 1 > n - k + 1$, as $k > n/2$. This is a contradiction since the spectral radius of B is $n - k - 1$. Hence $\lambda_1 = k$ and $\mu_1 = \rho(B)$. Thus if $i \geq 2$, then

$$|\lambda_i| = |\mu_i + 1| \leq |\mu_i| + 1 \leq n - k - 1 + 1 = n - k$$

This proves the first assertion.

Suppose there exists $i \geq 2$ such that $|\lambda_i| = n - k$. Thus $|\mu_i + 1| = n - k$, which implies either $\mu_i = n - k - 1$ or $-\mu_i = n - k + 1$. Notice the latter cannot hold since $\rho(B) = n - k - 1$. Hence there exists $i \geq 2$ such that $\mu_i = \rho(B)$. This implies that $\rho(B)$ is not a simple eigenvalue and therefore B is reducible (see [13] p. 508).

For the converse suppose B is reducible. It follows that B is the direct sum of $(0,1)$ matrices with line sums $n - k - 1$. Therefore there exists $i \geq 2$ so that $\mu_i = n - k - 1$, that is, $|\lambda_i| = n - k$. This proves the result. \square

In particular if $A \in G(n, k)$, with $k > n/2$, then any eigenvalue $\lambda \neq k$ of A satisfies $|\lambda| \leq n - k$. However, this bound on $\lambda \neq k$ is no longer tight in general, since A must also be nonsingular. For example, if $A \in G(7, 4)$, then $J - A - I$ is irreducible (see Example 3.1.1), and in fact, if λ is a subdominant eigenvalue of A , then it is easy to verify (by MATLAB) that $|\lambda| \leq 2.247 < 3$. Using Proposition 1.4.6 and Lemma 3.2.1, it follows that $J - (A(C_4) \oplus A(C_4)) - I \in G(8, 5)$, and it is readily verified that there exists a subdominant eigenvalue λ such that $\lambda = -3$, thus the bound is tight in this case.

4.4 Summary and Final Remarks

In this final section, we give a brief summary of the results presented in this thesis. We include for visual reference a table of the values of $M(n, k)$, $W(n, k)$,

$m(n, k)$ and $w(n, k)$ determined thus far. We also give some ideas for future research on the topic of this thesis.

In Chapter 2 we derived a formula for general n for $M(n, 2)$, see Corollary 2.1.8. We also determined in general $W(n, 2)$ and $w(n, 2)$, and in fact proved that $w(n, 2) = m(n, 2)$ and $W(n, 2) = M(n, 2)$, see Theorem 2.2.4. For general n we determined $M(n, n - 2)$, see Corollary 2.1.9.

In Chapter 3 we derived general formulae for $w(n, n - 3)$ and $W(n, n - 3)$, see Theorems 3.2.2 and 3.2.6. These results gave rise to new lower bounds for $M(n, 3)$ and $M(n, n - 3)$. In Chapter 1 we presented known upper bounds for $M(n, k)$, for all n, k . Throughout the thesis we determined $M(n, k)$, $W(n, k)$ and $w(n, k)$ for many specific cases of n and k , see also Table 4.1.

There remain many unanswered questions when $3 \leq k \leq n - 3$ for the extreme values discussed here. We have only lower and upper bounds for $M(n, k)$ when $k = 3$ or $n - 3$. Many of the results in Chapters 2 and 3 rely on the fact that $(0,1)$ matrices with constant line sums 2 or $n - 2$ can be decomposed into a simple block diagonal form. However, the situation for $(0,1)$ matrices with constant line sums k , where $3 \leq k \leq n - 3$, is vastly more complicated, and thus means for deriving formulae for $M(n, k)$ are more difficult. From Example 1.4.6 and Theorem 3.2.6, $M(7, 4) = 32 > W(7, 4) = 4$. This is the smallest value of $n + k$ where $M(n, k) \neq W(n, k)$ when $G(n, k) \neq \emptyset$. Applying similar arguments as in Example

1 4 9, and noting that the only disconnected graph on 8 vertices regular of degree 3 is $K_4 \cup K_4$, it follows that $W(8, 3) = 15$, whereas $w(8, 3) = 3$. We know only a bound for $M(8, 3)$, namely $M(8, 3) \geq 15$. Similarly using [7] Table 3 and Proposition 1 4 6, we can show that $W(8, 4) = 16$, thus $W(n, k)$ is determined for all n, k such that $n + k \leq 12$. However, $W(9, 4)$ is currently unknown. From the list of characteristic polynomials for all adjacency matrices of connected graphs on 12 vertices regular of degree 3 given in [7] Table 3, and using similar arguments as in Example 1 4 9, $W(12, 8) = 384$, and $w(12, 8) = 64 > m(12, 8) = 32$. This is the smallest value of $n + k$ where $w(n, k) \neq m(n, k)$ when $G(n, k) \neq \phi$. Using the general formulae and particular values given in this thesis, Table 4 1 summarizes results for $M(n, k)$, $W(n, k)$, $m(n, k)$ and $w(n, k)$ for $n \leq 12$.

n	k										
	1	2	3	4	5	6	7	8	9	10	11
2	1,1	*,*									
	1,1	*,*									
3	1,1	2,2	*,*								
	,	2,2	*,*								
4	1,1	*,*	3,3	*,*							
	1,1	*,*	3,3	*,*							
5	1,1	2,2	3,3	4,4	*,*						
	,	2,2	*,*	4,4	*,*						
6	1,1	4,4	9,9	8,8	5,5	*,*					
	1,1	4,4	*,*	*,*	5,5	*,*					
7	1,1	2,2	3,24	4,32	5,5	6,6	*,*				
	,	2,2	*,*	4,4	*,*	6,6	*,*				
8	1,1	4,4	3,?	16,?	5,?	12,12	7,7	*,*			
	1,1	4,4	3,15	16,16	5,15	*,*	7,7	*,*			
9	1,1	2,8	9,?	4,?	5,?	18,?	7,28	8,8	*,*		
	,	2,8	*,*	?,?	*,*	18,18	*,*	8,8	*,*		
10	1,1	4,4	3,?	8,?	25,?	12,?	7,?	16,16	9,9	*,*	
	1,1	4,4	3,48	?,?	?,?	12,192	7,21	*,*	9,9	*,*	
11	1,1	2,8	3,?	4,?	5,?	6,?	7,?	8,?	9,36	10,10	*,*
	,	2,8	*,*	?,?	*,*	?,?	*,*	8,24	*,*	10,10	*,*
12	1,1	4,16	9,?	16,?	5,?	36,?	7,?	32,?	27,?	20,80	11,11
	1,1	4,16	9,108	?,?	?,?	?,?	?,?	64,384	27,81	*,*	11,11

Table 4.1 Presently known values of $m(n, k)$, $M(n, k)$, $w(n, k)$ and $W(n, k)$ for $n \leq 12$

For each n, k the following values are given in each cell:

$$m(n, k), M(n, k)$$

$$w(n, k), W(n, k)$$

Here * indicates that the value does not exist, and ? indicates that the value is unknown.

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