Special Classes of Zero-One Matrices

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Abstract

We study two special classes of zero-one matrices. First, we consider matrices A satisfying $A^2 = J$. Short proofs are given for known results, new results and techniques are developed, and conjectures are settled. Second, we discuss two optimization problems through their relation to compound matrices and general combinatorial optimization techniques. Known results are discussed along with new perspectives on previously solved cases. Open cases are developed and both theoretical and computational techniques are extended. For both problems, many questions and conjectures are mentioned.

Chapter 1

Matrices A Satisfying $A^2 = J$

1.1 Introduction

A directed graph with n vertices is called a *central directed graph* (*central digraph*) if every pair of vertices are connected by a unique length 2 walk. (There may be walks of other lengths.) In terms of the adjacency matrix A of the graph, this happens precisely when $A^2 = J_n$, where J_n is the $n \times n$ matrix of all ones. In our discussion, we will let $\mathcal{A}_n$ be the set of all such matrices. It turns out that these concepts are related to the algebraic structure known as a *central groupoid*, which is a non-empty set S with n elements and a binary operation $*$ such that

$$(x * y) * (y * z) = y$$

for any elements x, y, z in the set. One can establish the correspondence between a central digraph and a central groupoid as follows. Identify the vertices of the graph with the elements in the groupoid so that $i * j = k$ if and only if $i \to k \to j$ is the unique length two walk from i to j.

Central digraphs, central groupoids and the matrix equation $A^2 = J_n$ have attracted the attention of many researchers in different areas because of their very rich and beautiful algebraic and combinatorial structures, and their connection to other pure and applied problems; e.g., see [9, 10, 14, 15] and their references.

In [9], Hoffman raised the question of finding all matrices in $\mathcal{A}_n$, which seems to be a very difficult problem. Nevertheless, many interesting properties and techniques have been discovered. The purpose of this work is to obtain more results on these subjects and to further develop techniques and insights in studying these concepts. In particular, we shall use approaches from algebra, combinatorial theory, matrix theory, and scientific computations. This chapter is organized as follows. In section 2, we reprove most of the basic results and obtain some new results on the subject. In section 3, we consider a simple operation for transforming a matrix in $\mathcal{A}_n$ to another matrix in $\mathcal{A}_n$. Using these operations we give a short proof for the interesting result of Shader [14] concerning the ranks of matrices in $\mathcal{A}_n$. In section 4, we study the row/column multiplicity conjecture of Fletcher on $\mathcal{A}_n$, and show that it is true if and only if $n = 1, 3, 9$. In section 5, we study sub-central groupoids, i.e., subsets of a central groupoid which are themselves central groupoids. To facilitate the study of central digraphs, several MatLab programs were developed. These programs are described in Section 6. Throughout the chapter, we will mention many open problems and conjectures.

Denote by $\{e_1, \ldots, e_k\}$ the standard basis for $\mathbf{R}^k$, with $e = e_1 + \cdots + e_k$. Then one can easily describe the *standard matrix* $A = (A_{ij})_{1 \le i,j \le k} \in \mathcal{A}_n$, where $n = k^2$ for some positive integer k and $A_{ij} = e_j e^t$ for $i, j \in \{1, \ldots, k\}$. For example, if $k = 3$, then $A = (A_{ij})_{1 \le i,j \le 3} \in \mathcal{A}_9$ with

$$A_{i1} = e_1 e^t = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \; A_{i2} = e_2 e^t = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \text{and} \quad A_{i3} = e_3 e^t = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{pmatrix}$$

for $i = 1, 2, 3$. When used below, the notation A will refer to an arbitrary matrix in $\mathcal{A}_n$ and not the standard matrix, unless specifically designated as such.

1.2 Basic Properties

The next two results are well-known. We include a short proof for the sake of completeness.

Theorem 1.2.1 *Let n be a positive integer. Then $\mathcal{A}_n \neq \emptyset$ if and only if $n = k^2$ for some positive integer k. Furthermore, if $n = k^2$ and $A \in \mathcal{A}_n$, then*

(a) *all row sums and column sums of A equal k,*

(b) *A has eigenvalues $k, 0, \ldots, 0$.*

(c) *A has exactly k 1's on its main diagonal.*

Proof. Suppose $n = k^2$. Then $A = (A_{ij})_{1 \le i,j \le k} \in \mathcal{A}_n$, where $A_{ij} = e_j e^t$ for $i, j \in \{1, \ldots, k\}$.

Conversely, suppose $\mathcal{A}_n$ is non-empty, and $A \in \mathcal{A}_n$. If A has row sums $r_1, \ldots, r_n$ and column sums $c_1, \ldots, c_n$, then $A^3 = AA^2 = AJ = (r_1, \ldots, r_n)^t (1, \ldots, 1)$ and $A^3 = A^2 A = JA = (1, \ldots, 1)^t (c_1, \cdots, c_n)$. Thus, all row sums and column sums are the same, say, equal to k. In particular, A has Perron root k with a positive (Perron) eigenvector $(1, \ldots, 1)^t$.

Now, since A^2 has eigenvalues $n, 0, \ldots, 0$, A has eigenvalues $\sqrt{n}, 0, \ldots, 0$, and hence $k = \sqrt{n}$. Since the trace of a matrix is equal to the sum of its eigenvalues, A has exactly k 1's on its main diagonal. □

Theorem 1.2.2 *The matrices in $\mathcal{A}_n$ have the following Jordan forms (all attainable):*

$$[\sqrt{n}] \oplus \underbrace{B \oplus \cdots \oplus B}_{p} \oplus 0_{n-2p-1} \qquad \textit{with} \qquad B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

and $\sqrt{n} - 1 \leq p \leq (n-1)/2$. Consequently, if $A \in \mathcal{A}_n$, then

$$\sqrt{n} \leq \operatorname{rank}(A) \leq (n+1)/2.$$

The first equality holds if and only if A is permutationally similar to the standard matrix $(A_{ij})_{1 \leq i,j \leq k}$, where $n = k^2$ and $A_{ij} = e_j e^t$ for $i, j \in \{1, \ldots, k\}$.

Proof. Since A^2 is diagonalizable with eigenvalues $n, 0, \ldots, 0$, the Jordan blocks of A corresponding to the eigenvalue 0 have size at most 2. Thus, the rank of A is at most $(n+1)/2$. By the result in [14] (see also Theorem 1.3.3 in the next section), all such ranks can be attained, and thus the prescribed Jordan structure can be attained.

Now, to prove the last assertion, note that AA^t has eigenvalues $k^2 = n = \lambda_1 \geq \cdots \geq \lambda_n \geq 0$, and $\operatorname{tr}(AA^t) = k^3$. It follows that AA^t has at least k positive eigenvalues. Moreover, if there are exactly k positive eigenvalues, each of them is equal to the Perron root k^2. So, there is a permutation matrix P such that $PAA^tP^t = A_1 \oplus \cdots \oplus A_k$, where each A_j has k^2 as the largest eigenvalue. Since each A_j has column sum and row sum k^2, we see that $A_j = k^2 J_k$ for $j = 1, \ldots, k$. Evidently, this happens if and only if PA has k groups of k identical rows, or equivalently, A is permutationally similar to the standard matrix. □

In the remainder of this section, we present several new results on $\mathcal{A}_n$. First, we present an additive decomposition of matrices in $\mathcal{A}_n$ in terms of permutation matrices. The following lemma will give some additional structure to the summands of the decomposition.

Lemma 1.2.3 *Let $A \in \mathcal{A}_n$ with $n = k^2$ for some positive integer k, and let $G(A)$ be the directed graph of A with vertices $v_1, \ldots, v_n$. Then k of the vertices in $G(A)$ have self loops, while all other vertices in $G(A)$ are paired in two-cycles, with no vertex belonging to more than one two-cycle.*

Proof. Since A has k 1's on its main diagonal, $G(A)$ has k self loops. No other vertex can be in a two-cycle with an idempotent vertex (that is, one with a self loop) since then there would be two length two walks from the idempotent vertex to itself. Since there must be a length two walk from each non-idempotent vertex to itself, the walk must be a two-cycle with two non-idempotent vertices. No vertex v_i can be in two two-cycles, say with v_j and v_k, since then there would be at least two length two walks from v_j to v_k. □

Theorem 1.2.4 *Let $n = k^2$ for some positive integer k. Every $A \in \mathcal{A}_n$ can be written as the sum of k permutation matrices, $A = P_1 + \cdots + P_k$, such that P_iP_j and P_rP_s have no common nonzero entries for any $(i, j) \neq (r, s)$ with $1 \leq i, j, r, s \leq k$. Moreover, we may assume that P_1 satisfies $P_1^2 = I_n$.*

Proof. By Corollary 1.2.5 in [3], A is the sum of k permutation matrices. Since $A^2 = J_n$, the condition on P_iP_j follows.

Finally, we assume that P_1 is the adjacency matrix corresponding to the loops and two cycles in Lemma 1.2.3. Then $P_1^2 = I_n$. □

A word $W(A, A^t)$ of length m is defined to be a product of m matrices $X_1, \ldots, X_m$ such that $X_j \in \{A, A^t\}$ for all j. The following theorem is new.

Theorem 1.2.5 *Suppose $A \in \mathcal{A}_n$, and $W(A, A^t)$ is a word of length m not of the form $(AA^t)^{m/2}$ or $(A^tA)^{m/2}$ when m is even. Then $W(AA^t)$ has eigenvalues $k^m, 0, \ldots, 0$.*

Proof. If $A^2 = J$ or $(A^t)^2 = J$ appears in $W(A, A^t)$, then $W(A, A^t) = k^{m-2}J$, and we are done. If not, $W(A, A^t)$ must be of the form $(AA^t)^{(m-1)/2}A$ or $(A^tA)^{(m-1)/2}A^t$ by our assumption. In both cases, we can shift the first letter to the last letter in the word to obtain a new word with the same eigenvalues. The result now follows from the first case. □

Recall that the permanent of $A = (a_{ij})$ is denoted and defined by per $(A) = \sum_\sigma \prod_{j=1}^n a_{j\sigma(j)}$, where σ ranges through all possible permutation of $(1, \ldots, n)$. The permanent of a $(0, 1)$ matrix A can be viewed as the number of permutation matrices P such that $A - P$ is nonnegative. This is useful topic in combinatorial analysis; e.g., see [3, Chapter 7]. In connection to our study, we have the following result:

Theorem 1.2.6 *Let $A \in \mathcal{A}_n$, where $n = k^2$ for some positive integer k. Then* per $(A) \leq$ *$(k!)^k$, where the equality holds if and only if* rank $(A) = k$.

Proof. See [1] and Theorem 7.4.7 in [3]. □

Problem 1.2.7 It would be interesting to determine all possible eigenvalues of AA^t and all possible $\operatorname{per}(A)$ values with $A \in \mathcal{A}_n$.

1.3 Transforming Matrices in $\mathcal{A}_n$ by Switches

Suppose $(i_1, \cdots, i_k)$ and $(j_1, \ldots, j_k)$ are subsequences of $(1, \ldots, n)$. Denote by

$$A[i_1, \ldots, i_k; j_1, \ldots, j_k]$$

the submatrix of A lying in rows $i_1, \ldots, i_k$, and columns $j_1, \ldots, j_k$. We have the following observation.

Theorem 1.3.1 *Let $A \in \mathcal{A}_n$, $1 \leq p < q \leq n$, and $1 \leq r < s \leq n$ satisfy*

$$A[p, q; r, s] \in \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\}.$$

Suppose $\tilde{A}$ is obtained from A by replacing $A[p, q; r, s]$ with $J_2 - A[p, q; r, s]$. Then $\tilde{A} \in \mathcal{A}_n$ if and only if $\{p, q\} \cap \{r, s\} = \emptyset$, rows r and s of A are the same, and columns p and q of A are the same. Moreover, the ranks of $\tilde{A}$ and A can differ at most by one.

Proof. The first assertion follows readily from simple graph considerations; see [5]. For the second assertion, note that $\tilde{A} - A = \pm(e_p - e_q)(e_r - e_s)^t$, and thus the ranks of $\tilde{A}$ and A can differ at most by one. □

If $\tilde{A} \in \mathcal{A}_n$ is obtained from A by a change described in the above proposition, we say that $\tilde{A}$ is obtained from A by a *switch*. The following conjecture is mentioned in [5] (see also [6]).

Conjecture 1.3.2 Every $A \in \mathcal{A}_n$ can be obtained from the standard matrix by a finite number of switches.

While we are not able to prove or disprove the above conjecture, we are able to use the concept of a switch to give a short proof of the interesting result in [14], namely, there are matrices in $\mathcal{A}_n$ with rank r if and only if $\sqrt{n} \leq r \leq (n+1)/2$. In Theorem 1.3.3, we will describe how one can use switches to transform the standard matrix in $\mathcal{A}_n$ to a matrix with maximum rank such that the rank of the matrix is increased by one in each step. In the following, we will denote a switch by $[p, q; r, s]$, and the basic circulant by $T_k = [e_k|e_1|e_2|\cdots|e_{k-1}]$; e.g.,

$$T_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; T_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \; T_4 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Theorem 1.3.3 *Suppose $k \geq 3$ is a positive integer and $n = k^2$, and $A = (A_{ij})_{1\leq,i,j\leq k}$ such that $A_{ij} = e_j e^t \in M_k$ for $i, j \in \{1, \ldots, k\}$. Consider the following three types of switches:*

(1) *$(k-2)$ switches in the submatrix $[A_{11}|A_{12}|\cdots|A_{1k}]$ as follows:*

$[2, 3; k+3, 2k+3]$,

$[3, 4; 2k+4, 3k+4]$,

$[4, 5; 3k+5, 4k+5]$,

$\vdots \quad \vdots \quad \vdots$

$[k-2, k-1; (k-3)k + (k-1), (k-2)k + (k-1)]$,

$[k-1, k; (k-2)k + k, (k-1)k + k]$.

(2) *For $k \geq 4$, $(k-2)(k-3)/2$ switches in the submatrices $[A_{i1}|A_{i2}|\cdots|A_{ik}]$ for $i = 4, \ldots, k$ as follows. For $i = 4, \ldots, k$, we have $(i-3)$ switches:*

$[(i-1)k + 2, (i-1)(k+1); k+i, (i-2)k + i]$,

$[(i-1)k + 2, (i-1)k + 3; 2k+i, (i-2)k + i]$,

$[(i-1)k + 3, (i-1)k + 4; 3k+i, (i-2)k + i]$,

$\vdots \quad \vdots \quad \vdots$

$[(i-1)k + (i-3), (i-1)k + (i-2); (i-3)k + i, (i-2)k + i]$

(here ignoring the first switch, one has an easy pattern for the other $i-4$ switches) that transform the submatrix I_{i-2} in rows indexed $2, \ldots, i-1$ and columns indexed by $k+i, 2k+i, \ldots, (i-2)k+i$ of $[A_{i1}|A_{i2}|\cdots|A_{ik}]$ to T_{i-2}.

For example, there is 1 switch for $i = 4$: $[3k+2, 3k+3; k+4, 2k+4]$; there are 2 switches for $i = 5$: $[4k+2, 4k+4; 1k+5, 3k+5]$, $[4k+2, 4k+3; 2k+5, 3k+5]$; there are 3 switches for $i = 6$: $[5k+2, 5k+5; 1k+6, 4k+6]$, $[5k+2, 5k+3; 2k+6, 4k+6]$, $[5k+3, 5k+4; 3k+6, 4k+6]$.

(3) $[(k-1)/2]$ *switches in the submatrices* $[A_{i1}|A_{i2}|\cdots|A_{ik}]$ *for* $i = 3, 5, 7, \ldots$ *as follows:*

$[2k+1, 2(k+1); 1, k+1]$,

$[4k+1, 4(k+1); 1, 3k+1]$,

$\vdots \quad \vdots \quad \vdots$

$[2mk+1, 2m(k+1); 1, (2m-1)k+1]$, *where* $m = [(k-1)/2]$.

If A is modified by consecutively applying the above switches, then the following conditions hold:

(a) *Every switch is legal, i.e., the matrix remains in $\mathcal{A}_n$ after every switch.*

(b) *Every switch increases the rank of the current matrix by one, and the final matrix has rank $[n/2]$.*

Proof. To prove part (a), note that by Theorem 1.3.1, a switch $[p, q; r, s]$ may be legally performed on a matrix $B \in \mathcal{A}_n$ if and only if $\{p, q\} \cap \{r, s\} = \emptyset$, row r and row s of B are identical, and column p and column q of B are identical.

In the proposed switches, rows with the following indices will be changed:

Type (1) switches: $2, \ldots, k$,

Type (2) switches:

$$\begin{array}{l} 3k+2, 3k+3 \\ 4k+2, 4k+3, 4k+4, \\ 5k+2, 5k+3, 5k+4, 5k+5, \\ \quad \vdots \quad \vdots \quad \vdots \\ (k-1)k+2, (k-1)k+3, \ldots, (k-1)k+(k-1). \end{array}$$

Type (3) switches:

$$\begin{array}{l} 2k+1, 2(k+1) \\ 4k+1, 4(k+1) \\ 6k+1, 6(k+1) \\ \quad \vdots \quad \vdots \quad \vdots \\ 2mk+1, 2m(k+1). \end{array}$$

Also, columns with the following indices will be changed:

Type (1) switches:

$$\begin{array}{l} k+3 \\ 2k+3, 2k+4, \\ 3k+4, 3k+5, \\ \quad \vdots \quad \vdots \quad \vdots \\ (k-2)k+(k-1), (k-2)k+k, \\ (k-1)k+k. \end{array}$$

Type (2) switches:

$$\begin{array}{l} k+4, 2k+4 \\ k+5, 2k+5, 3k+5, \\ \quad \vdots \quad \vdots \quad \vdots \\ k+(k-1), 2k+(k-1), \ldots, (k-3)k+(k-1). \\ k+k, 2k+k, \ldots, (k-2)k+k. \end{array}$$

Type (3) switches: $1, k+1, 3k+1, \ldots, (2m-1)k+1$.

Note that the two lists of indices corresponding to row changes and columns changes are disjoint. Hence, for each proposed switch $[p, q; r, s]$, no matter how many other proposed switches have already been performed, columns p and q have not been changed and they are identical to columns p and q in the original matrix A, which are equal; similarly, rows r and s have not been changed throughout the process and thus are identical to rows r and s in the original matrix A, which are equal. Therefore, all the proposed switches are legal.

Despite this simple proof of (a), one may want to trace the pattern of how the list of the forbidden (for use in switches) row and columns indices grows throughout the process, but still leaves an adequate number of equal rows and equal columns for future switches.

To prove (b), note that the total number of proposed switches equals

$$(k-2)+(k-2)(k-3)/2+[(k-1)/2] = (k-1)(k-2)/2+[(k-1)/2].$$

Since every switch can only increase rank by at most one, the final matrix has rank not larger than

$$k+(k-1)(k-2)/2+[(k-1)/2] = \begin{cases} (k^2+1)/2 & \text{if } k \text{ is odd,} \\ k^2/2 & \text{if } k \text{ is even,} \end{cases}$$

which is $[(n+1)/2]$. Thus, we need only to show that the final matrix has rank $[(n+1)/2]$; it will then follow that each proposed switch indeed increases the rank by one. To achieve our goal, we show that the row space of the final matrix contains $[(n+1)/2]$ linearly independent vectors.

First, pick the k rows in $[A_{21}|A_{22}|\cdots|A_{2k}]$, which have not been changed at all. Denote these row vectors by $u_1, \ldots, u_k$. Note that the column indices of the leading ones of these row vectors are:

$$1, k+1, 2k+1, \ldots, (k-1)k+1.$$

Next, pick the $(k-2)$ rows that resulted from the type (1) switches, namely, those rows indexed by $3, 4, \ldots, k$. Denote these row vectors by $v_1, \ldots, v_{k-2}$. Note that the column indices of the leading ones of these rows are:

$$k+3, 2k+4, 3k+5, \ldots, (k-2)k+k.$$

Now, consider the rows that resulted from the type (2) switches in $[A_{i1}|\cdots|A_{ik}]$ for $i = 4, \ldots, k$.

For $i = 4$, consider the row indexed by $3k+2$ in the final matrix. Subtracting this vector from u_2 (the second row of $[A_{21}|\cdots|A_{2k}]$), we get a row vector with leading one at the $(k+4)$th position. Denote this vector by w_1.

For $i = 5$, consider the rows indexed by $4k+2$ and $4k+3$ in the final matrix. Subtracting these vectors from u_2 and u_3 (the second and third row of $[A_{21}|\cdots|A_{2k}]$), respectively, we get two row vectors with leading ones at the positions indexed by $k+5, 2k+5$. Denote these vectors by w_2 and w_3.

For $i = 6$, consider the rows indexed by $5k+2$, $5k+3$, and $5k+4$ in the final matrix. Subtracting these vectors from u_2, u_3 and u_4, respectively, we get three row vectors with leading ones in the positions indexed by $k+6, 2k+6, 3k+6$. Denote these vectors by w_4, w_5 and w_6.

Continuing the above method, we obtain vectors $w_1, \ldots, w_r$ in the row space of the final matrix, where $r = (k-2)(k-3)/2$, and the leading ones of these vectors are in the positions:

$$\begin{array}{l} k+4, \\ k+5, 2k+5, \\ k+6, 2k+6, 3k+6, \\ \quad\;\;\vdots \quad\;\; \vdots \\ 2k, 3k, \ldots, (k-2)k. \end{array}$$

Finally, consider the following row vectors in the final matrix that resulted from type (3) switches, namely, those rows indexed by

$$2k+1, 4k+1, 6k+1, \ldots, 2mk+1,$$

where $m = [(k-1)/2]$. Let $z_1, \ldots, z_m$ be these row vectors. Let $x_1 = z_m$ and $x_{j+1} = z_{j+1} - z_j + u_{2j}$ for $j = 1, \ldots, m-1$. Then $x_1, \ldots, x_m$ are vectors in the row space of the final matrix, and their leading ones lie in the positions indexed by

$$2, k+2, 3k+2, 5k+2, \ldots, (2m-3)k+2.$$

Now, consider the vectors

$$u_1, \ldots, u_k, v_1, \ldots, v_{k-2}, w_1, \ldots, w_r, x_1, \ldots, x_m$$

in the row space of the final matrix. Since their leading ones all lie in different positions, we have a linearly independent set of size $[(n+1)/2]$ as desired. $\square$

In the following, we exhibit the matrices with maximum rank in $\mathcal{A}_{16}$ and $\mathcal{A}_{25}$ obtained using our scheme. For easy reference, we highlight the entries involved in the switches we applied. One can follow our proof to identify the basis for the row space in each case.

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

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

Next, we consider different matrices in $\mathcal{A}_n$ that can be obtained by one switch.

Proposition 1.3.4 *Suppose $n = k^2 \geq 16$. Then up to permutation similarity, there are four different matrices obtained from the standard matrix by applying one switch.*

Proof. Let $A \in \mathcal{A}_n$ be the standard matrix. Assume the switch take place at $A[p, q; r, s]$. We consider two cases. First, row r or row s contains a nonzero diagonal entry. In this case, we may apply a permutation similarity and assume that $r = 1$ and $s = k + 1$. Since column p and column q are identical, there exists $m \in \{1, \ldots, k\}$ such that $(m-1)k < p, q \leq mk$. Now, it is easy to check that $m \neq 1, 2$. If $m \geq 3$, then we may assume that $m = 3$; otherwise, apply a permutation similarity involving row and column indices at least $2k$ to A. Now, in order to have

$$A[p, q; r, s] \in \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\},$$

we see that $p = 2k + 1$ and $2k + 1 < q \leq 3k$. Up to permutation similarity, we may assume that $q = 2k + 2$. So, up to permutation similarity, there is only one matrix with the desired property in this case.

Case 2. Neither row r nor row s contains a nonzero diagonal entry. By permutation similarity, we may assume that $r = 2$ and $s = k + 2$. Since column p and column q are identical, there exists $m \in \{1, \dots, k\}$ such that $(m - 1)k < p, q \leq mk$. It is now easy to check that, up to permutation similarity, there is one desired matrix with $m = 1$, say, with $(p, q) = (1, 3)$; one matrix with $m = 2$, say, with $(p, q) = (k + 1, k + 3)$; one matrix with $m \geq 3$, say, with $(m, p, q) = (3, 2k + 1, 2k + 2)$. So, up to permutation similarity, there are three matrices of the desired form in this case.

Combining, up to permutation similarity, there are four matrices that differ by one switch from the standard matrix. □

The previous proposition naturally leads to the following related problem:

Problem 1.3.5 Find all matrices that can be obtained by applying two switches to the standard matrix.

Since we need identical rows and identical columns to perform switches, it would also be helpful to resolve the following question:

Problem 1.3.6 Are there always identical rows and identical columns for matrices in $\mathcal{A}_n$?

1.4 Row and Column Multiplicities

A matrix $A \in \mathcal{A}_n$ is said to have row multiplicities $m_1 \geq m_2 \geq \cdots \geq m_s$ if A has m_1 rows that are equal, m_2 other rows that are equal, etc., where $m_1 + m_2 + \cdots + m_s = n$. Similarly we can define the column multiplicities of A.

R.R. Fletcher III conjectured (see [5], [6]) that for each A such that $A^2 = J$, the multisets of integers representing the column and row multiplicities of A are equal. We have settled his conjecture by the following result:

Theorem 1.4.1 *Suppose $n = k^2$ for some positive integer k. If $k \leq 4$ and $A \in \mathcal{A}_n$, then the row and column multiplicities of A are the same. If $k \geq 4$, there there is an $A \in \mathcal{A}_n$ whose row and column multiplicities are different.*

Proof. If $n = 1, 4$, the result is clear. If $n = 9$, the result is true by the comment in [10] or Proposition 1.4.2. Suppose $n = k^2 \geq 16$. Consider $A = (A_{ij})_{1 \leq i,j \leq k}$ such that $A_{i1} = e_1(e_1 + e_k)^t + e_2(e_2 + \cdots + e_{k-1})^t$ and $A_{i2} = e_2(e_1 + e_k)^t + e_1(e_2 + \cdots + e_{k-1})^t$ for

$i = 1, \ldots, k-1$, and $A_{ij} = e_j e^t$ for all other $i, j \in \{1, \ldots, k\}$. Then A has row multiplicities $\underbrace{k, \ldots, k}_{k-2}, k-1, k-1, 1, 1$, and column multiplicities $\underbrace{k, \ldots, k}_{k-2}, k-2, k-2, 2, 2$. The result follows. □

For example, when $k = 4$, the construction in the above proof yields

$$\begin{bmatrix} B_1 & B_2 & A_3 & A_4 \\ B_1 & B_2 & A_3 & A_4 \\ B_1 & B_2 & A_3 & A_4 \\ A_1 & A_2 & A_3 & A_4 \end{bmatrix}, \quad \text{where} \quad B_1 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and $A_j = e_j e^t$ for $j = 1, \ldots, 4$. This matrix has row multiplicities {4,4,3,3,1,1} and column multiplicities {4,4,2,2,2,2}.

Proposition 1.4.2 *Up to permutation similarity, $\mathcal{A}_9$ consists of the following six different matrices:*

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

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

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

Proof. Suppose $A \in \mathcal{A}_9$. Let B be the 6-by-9 matrix formed by deleting the last 3 rows of A, and let C be the 6-by-9 matrix formed by deleting rows 4, 5 and 6 of A. We may assume by permutation similarity that A has the form $(A_{ij})_{1\le i,j\le 3}$, where

$$A_{11} = \begin{pmatrix} 1&1&1\\ 0&0&0\\ 0&0&0 \end{pmatrix},\ A_{12} = \begin{pmatrix} 0&0&0\\ 1&1&1\\ 0&0&0 \end{pmatrix},\ A_{13} = \begin{pmatrix} 0&0&0\\ 0&0&0\\ 1&1&1 \end{pmatrix}.$$

Further, we may assume that $\operatorname{rank}(B) \ge \operatorname{rank}(C)$ since, if not, rows (and columns) 4, 5 and 6 of A can be interchanged with rows (and columns) 7, 8 and 9, and then rows (and columns) 2 and 3 of A can be interchanged, thus maintaining the desired form for the first 3 rows of A and yielding the desired inequality between the ranks of B and C.

We will find all solutions to $A^2 = J$ by considering the possible ranks of B. Denote row i and column i of A by r_i and c_i respectively, for $i = 1, \ldots, n$. Since $r_1 + r_2 + r_3 = r_4 + r_5 + r_6$, the rows of B are dependent and hence $3 \le \operatorname{rank}(B) \le 5$. Clearly, if $\operatorname{rank}(B) = 3$, then $\operatorname{rank}(A) = 3$ and A can have no row that differs from one of its first three rows. It follows easily that if $\operatorname{rank}(B) = 3$, then A satisfies (or can have its rows and columns permuted to satisfy) $A_{11} = A_{21} = A_{31}$, $A_{12} = A_{22} = A_{32}$, and $A_{13} = A_{23} = A_{33}$. We must now consider solutions for which $\operatorname{rank}(B)$ is equal to 4 or 5.

Let A be a solution such that $\operatorname{rank}(B) = 4$ or 5. Since the submatrix A_{21} contains three 1's, there are three cases to consider:

1) Each row of A_{21} contains exactly one 1,

2) One row of A_{21} contains exactly two 1's, and

3) All three 1's lie in one row of A_{21}.

In case 1) we may assume by permutation similarity that $A_{21} = I_3$. Since $r_4c_1 = 1$, $a_{44} = 0$. Similarly, since $r_4c_2 = 1$ and $r_4c_3 = 1$, $a_{45} = 0$ and $a_{46} = 0$. Because $r_5c_5 = 1$, $a_{55} = 0$. Since each column of A_{22} contains exactly one 1, $a_{65} = 1$. Then $r_6c_7 = r_6c_8 = r_6c_9 = 1$ implies that the second row of A_{23} is $(0, 0, 0)$. Since r_5 contains exactly three 1's, the second row of A_{22} is $(1,0,1)$ and thus $r_5c_5 \geq 2$, which is not possible. Hence there are no solutions in case 1).

In case 2) we may assume that row one of A_{21} is $(1,1,0)$, $(1,0,1)$, or $(0,1,1)$ and that row three of A_{21} is $(0,0,0)$. If row one of A_{21} is $(1,1,0)$, then row one of A_{22} must be $(0,0,0)$ or $(0,0,1)$, as will be shown in the following paragraph. In the former case there is one solution with $\operatorname{rank}(A) = \operatorname{rank}(B) = 4$ and one solution with $\operatorname{rank}(B) = 4$ and $\operatorname{rank}(A) = 5$. In the latter case there are two solutions with $\operatorname{rank}(A) = \operatorname{rank}(B) = 4$ and one solution with $\operatorname{rank}(B) = 4$ and $\operatorname{rank}(A) = 5$.

We now verify the above claim that if row one of A_{21} is $(1,1,0)$ and row two is $(0,0,1)$, then row one of A_{22} must be $(0,0,0)$ or $(0,0,1)$. We also show that if row one of A_{22} is $(0,0,0)$, then a single solution with $\operatorname{rank}(A) = \operatorname{rank}(B) = 4$ results. Other cases in this section can be examined in a similar manner. Since $r_4c_1 = 1$, $a_{44} = 0$. Similarly $a_{45} = 0$ since $r_4c_3 = 1$. Thus row one of A_{22} is either $(0,0,0)$ or $(0,0,1)$. Suppose the former. Since r_4 contains three 1's, we may assume that the first row of A_{23} is $(1,0,0)$. Since $\operatorname{rank}(A) = 4$, $r_4 + r_5 = r_1 + r_3$ and hence the second row of A_{23} is $(0,1,1)$. Then the third row of A_{22} must be $(1,1,1)$. Since $r_4A = e$, the first row of A_{33} is $(1,1,1)$, implying $r_8 + r_9 = r_1 + r_2$. Because $\operatorname{rank}(A) = 4$, r_8 and r_9 must belong to the set $r_1, \ldots, r_6$ and hence must be r_1 and r_2, thus verifying the existence of a unique solution in this case.

Continuing case 2), if row one of A_{21} is $(1,0,1)$ and $\operatorname{rank}(B) = 4$, then it follows that the first two rows of A_{23} are $(1,0,0)$ and $(0,1,1)$, which results in two solutions. If row one of A_{21} is $(1,0,1)$ and $\operatorname{rank}(B) = 5$, there is one solution. Concluding case 2), if row one of A_{21} is $(0,1,1)$ and $\operatorname{rank}(B) = 4$, then the first two rows of A_{23} are $(0,0,1)$ and $(1,1,0)$, which yields one solution. If row one of A_{21} is $(0,1,1)$ and $\operatorname{rank}(B) = 5$, there is one solution.

In case 3) we may assume that the three 1's lie in the first row of A_{21}. Since no row of A_{22} contains three 1's, we may also assume that row two of A_{22} contains exactly two 1's, being equal to $(1,1,0)$, $(1,0,1)$, or $(0,1,1)$. The first two possibilities yield one solution each while the third possibility yields two solutions. All four of these solutions have the property that $\operatorname{rank}(A) = \operatorname{rank}(B) = 4$.

The cases considered above yield all possible solutions to $A^2 = J$ for $n = 9$. Fifteen solutions have been produced, but it is required that no two solutions be permutation similar. Using a Matlab program described in Section 6, we see that only six solutions remain. $\square$

A similar analysis to find the matrices in $\mathcal{A}_{16}$ seems prohibitively difficult (see [4]).

1.5 Sub-Central Groupoids

A proper subset of a central groupoid is called a *sub-central groupoid* if the subset is itself a central groupoid, using the same binary operation. In terms of matrices, if the initial central groupoid is of size k^2, then a sub-central groupoid corresponds to a principal submatrix B of a matrix $A \in \mathcal{A}_{k^2}$ such that $B \in \mathcal{A}_{r^2}$, for some natural number $r < k$. First, we show that every central groupoid of size k^2 can be embedded in a central groupoid of size $(k+1)^2$.

Theorem 1.5.1 *Suppose $A \in \mathcal{A}_{k^2}$ for some positive integer k. Then there exists a $k^2 \times k^2$ permutation matrix R and $k \times k$ permutation matrices $P_1, \ldots, P_k$ with $P_1 = I_k$ such that*

$$\tilde{A} = \begin{pmatrix} R^tAR & P & O_{k^2,k+1} \\ O_{k+1,k^2} & O_{k+1,k} & J_{k+1} \\ Q & I_k & O_{k,k+1} \end{pmatrix} \in \mathcal{A}_{(k+1)^2}$$

and $\operatorname{rank}(\tilde{A}) = \operatorname{rank}(A) + 1$*, where*

$$P = \begin{pmatrix} P_1 \\ \vdots \\ P_k \end{pmatrix} \qquad and \qquad Q = [e_1e^t|\cdots|e_ke^t].$$

Proof. First, let R be a $k^2 \times k^2$ permutation matrix such that $R^tAR = (A_{ij})_{1\le i,j\le k}$, where all A_{ij} are $k \times k$ and $A_{1j} = e_je^t$ for $j = 1, \ldots, k$. Considering the first k rows of the equation $J_{k^2} = (R^tAR)^2$, we see that every column in A_{ij} has exactly one nonzero entry. Also, there is a permutation matrix S such that $S^{-1}(R^{-1}AR)S = (B_{ij})_{1\le i,j\le k}$, where all B_{ij} are $k \times k$ and $B_{ij} = ee_i^t$ for $j = 1, \ldots, k$. Now, let $B = (B_{i1})_{1\le i\le k}$ and $P = S^{-1}B$. Then P consists of k columns of $R^{-1}AR$, whose sum is equal to the $k^2 \times 1$ vector with all entries equal to one. Partition the matrix $P = (P_{i1})_{1\le i\le k}$ so that each P_{i1} has size k. Since every column of A_{ij} has exactly one nonzero entry, every column of P_{i1} has at most one nonzero entry. Since the sum of the columns of P is the vector with all ones, we see that each row and column of P_{i1} has exactly one nonzero entry. Hence P_{i1} is a permutation matrix for all $i = 1, \ldots, k$. We may permute the columns of P so that $P_{i1} = I_k$. Then append the additional rows and columns to construct $\tilde{A}$. One can check that $\tilde{A}^2 = J_{(k+1)^2}$, say, by showing $v\tilde{A}$ is the vector of all ones for each row vector v of $\tilde{A}$.

Note that appending P to A will not increase the rank of the matrix because columns of P are chosen from those of R^tAR. Then appending the columns

$$\begin{pmatrix} O_{k^2,k+1} \\ J_{k+1} \end{pmatrix}$$

will increase the rank by one. Finally, appending the last k rows of $\tilde{A}$ will not further increase the rank because these rows are the same as the first k rows. Combining the arguments, we see that $\text{rank}\,(\tilde{A}) = \text{rank}\,(A) + 1$. □

We have the following conjecture.

Conjecture 1.5.2 Let k be a positive integer. Every central groupoid of size k^2 has a sub-central groupoid of size $(k-1)^2$.

Note that if this conjecture is true, then every central groupoid of size k^2 can be built from a central groupoid of size $(k-1)^2$. With the help of a computer, we can verify the conjecture for $k = 2, 3$. The general case remains open. Nonetheless, we have the following:

Theorem 1.5.3 *Every central groupoid of size k^2 has at most k different sub-central groupoids. This upper bound is attained by the standard central groupoid, i.e., the one whose corresponding matrix is the standard matrix.*

Proof. We prove the result using the central digraph and sub-central digraph language.

By Lemma 1.2.3, for every central digraph with $n = k^2$ vertices, there are k vertices with self-loops and the other $k(k-1)/2$ vertices are paired into disjoint two-cycles. Thus, if the central digraph has a sub-central digraph with $(k-1)^2$ vertices, it must be obtained by removing one vertex with a self-loop, and $2(k-1)$ vertices lying in $(k-1)$ two-cycles.

To prove our first assertion, we show that for each vertex v with a self-loop one can have at most one sub-central diagraph not containing the vertex v. Suppose there is indeed a sub-central digraph not containing the vertex v with a self-loop. Let $u_1, \ldots, u_{k-1}$ and $w_1, \ldots, w_{k-1}$ be vertices such that (u_j, v) and (v, w_j) are edges in the directed graph for $j = 1, \ldots, k-1$. We will say that the u_j's are *incoming vertices* of v and the w_j's are *outgoing vertices* of v.

Case 1. If $u_1, \ldots, u_{k-1}, w_1, \ldots, w_{k-1}$ are the vertices of $(k-1)$ two-cycles, then the resulting sub-central digraph must use all the remaining vertices.

Case 2. If an incoming vertex of v, say, u_1, remains in the sub-central digraph, then none of the w_j can be in the sub-central digraph. Othwise, there will be no length two walk from u_1 to the vertex w_j. Note that (w_i, w_j) cannot be an edge in the central digraph. Otherwise, there will be two walks from v to w_j, namely, $v \to v \to w_j$ and $v \to w_i \to w_j$. So, the sub-central digraph must use the vertices not involving v and the vertices in the $(k-1)$ two-cycles containing $w_1, \ldots, w_{k-1}$. In particular, u_1 cannot be a vertex in these two-cycles. So, we see that Case 2 and Case 1 cannot happen simultaneously.

Case 3. If an outgoing vertex of v remains in the sub-central digraph, then by arguments similar to Case 2, none of the u_j can be in the sub-central digraph, and the sub-central digraph must use the vertices not involving v and the vertices in the $(k-1)$ two-cycles containing $u_1, \ldots, u_{k-1}$. Again, Case 1 and Case 3 cannot overlap.

To finish the proof of our claim, we need to show that Case 2 and Case 3 cannot overlap. Then every self-loop vertex v can only associate with a sub-central digraph corresponding to one of Case 1, Case 2, or Case 3. Consequently, there will be at most k sub-central digraphs for the given central digraph.

Now, suppose Case 2 holds. We can label the vertices of the central digraph so that vertex 1 has a self-loop and vertices $2, \ldots, k$ are the outgoing vertices from vertex 1. We may assume that the adjacency matrix $A \in \mathcal{A}_n$ has block form $A = (A_{ij})_{1 \le i,j \le k}$, where A_{ij} are $k \times k$ and

$$[A_{11}| \cdots |A_{1k}] = [e_1 e^t| \cdots |e_k e^t].$$

Furthermore, we may label the other vertex in the two-cycle involving vertex j as $(j-1)k+1$ for $j = 2, \ldots, k$. Then

$$A_{ij} = \begin{pmatrix} * & * \\ * & B_{i-1,j-1} \end{pmatrix}, \quad i,j \ge 2,$$

in which $(B_{rs})_{1 \le r,s \le k-1} \in \mathcal{A}_{(k-1)^2}$ is the adjacency matrix of the the sub-central digraph obtained by removing vertex 1 and the $2(k-1)$ vertices corresponding to the two-cycles containing the vertices $2, \ldots, k$. Since the column sums of B are all $k-1$, the column sums of A are all k, and $[A_{11}| \cdots |A_{1k}] = [e_1 e^t| \cdots |e_k e^t]$, we see that the first row of A_{ij} have the form $[* \ O_{1,k-1}]$ for $i, j \in \{2, \ldots, k\}$.

Next, we claim that

$$A_{i1} = \begin{pmatrix} * & J_{1,k-1} \\ * & O_{k-1} \end{pmatrix}, \quad i = 2, \ldots, k.$$

Since $A^2 = J$ and $[A_{11}| \cdots |A_{1k}] = [e_1 e^t| \cdots |e_k e^t]$, we see that each column of A_{ij} has exactly one nonzero entry. Suppose $i \ge 2$ and the (r, s) entry of A_{i1} is nonzero for some $r, s \in \{2, \ldots, k\}$. Then there will be two length 2 walks from vertex $((i-1)k + r)$ to vertex sk, namely, $((i-1)k + r) \to s \to sk$, and a walk via a vertex in the sub-central digraph corresponding to the matrix B. This is a contradiction. So, all the rows with indices $(i-1)k + r$ have the form $[*, 0, \ldots, 0]$ for $i, r \in \{2, \ldots, k\}$. Since each column of A_{i1} has column sum 1, we see that the first row of A_{i1} has the form $[*, 1, \ldots, 1]$ as asserted.

If the first row of A_{p1} does not equal e^t for $p = 1, \ldots, k$, we are back to Case 1, namely, the vertices to be removed to produce the sub-central digraph will be self-loop vertex 1 and the $k-1$ pairs of two-cycle vertices $j, (j-1)k+1$ for $j = 2, \ldots, k$. So, there exists $p \geq 2$ such that the first row of A_{p1} equals $[0, 1, \ldots, 1]$. We may permute the rows and columns with indices $(p-1)k+2, \ldots, pk$ so that the $(2,1)$ entry of A_{p1} is nonzero. Thus, in A_{p1} the first row equals $[0, 1, \ldots, 1]$, and the second row equals $[1, 0, \ldots, 0]$ and all other rows are zero. Since all the row sums of A equal k, we see that there is $q > 1$ such that the first row of A_{pq} equals $[1, 0, \ldots, 0]$. Clearly, $p \neq q$; otherwise, we get an extra self-loop vertex (in addition to vertex 1, and the $k-1$ self-loop vertices in the submatrix B). Considering the product of the $((p-1)k+1)$st row and the first column of A, we see that the $(1,1)$ entry of A_{q1} must equal one.

Now, we can show that Case 3 cannot hold. If it does, then one can remove vertex 1, and the vertices of the two-cycles involving the incoming vertices of 1. In particular, we will remove vertex 1 and vertex $(q-1)k+1$. After this removal, columns with indices $2, \ldots, k$ will have column sums at most $k-2$. So, these columns cannot appear in the adjacency matrix of the sub-central digraph. Removing these columns, we see that all the rows with indices $ik+1$ for $i = 1, \ldots, k-1$ will have row sum at most 1 in the remaining matrix. Thus, they cannot appear in the adjacency matrix of the sub-central digraph. Combining, we have removed vertices $1, 2, \ldots, k$, and $ik+1$ for $i = 1, \ldots, k-1$. Together with the incoming vertex $(p-1)k+2$, we must remove at least $2k$ vertices, which is impossible. Hence, we have proved the first assertion of the theorem.

Now, suppose we have the standard central groupoid, and let $A \in \mathcal{A}_n$ be the corresponding matrix. For any self-loop vertex, we can find a suitable permutation matrix P so that the vertex appears as vertex n in the graph of the adjacency matrix $P^tAP \in \mathcal{A}_n$, which is again in standard form. Now, removing the rows and columns indexed by $k, 2k, \ldots, k^2$, we produce a sub-central groupoid. Since this works for each vertex with a self-loop, we get k distinct sub-central digraphs. □

From the proof of the above theorem, we see that if $A \in \mathcal{A}_{k^2}$ has a principal submatrix $B \in \mathcal{A}_{(k-1)^2}$, then A has a row or a column with multiplicity at least $k-1$. As a result, if Conjecture 1.5.2 is true, then we have:

Conjecture 1.5.4 Every $A \in \mathcal{A}_{k^2}$ has a row or a column with multiplicity at least $k-1$.

Settling this conjecture positively would solve Problem 1.3.6, which asks if there are always identical rows and columns for matrices in $\mathcal{A}_{k^2}$. Note also that it is not true that every $A \in \mathcal{A}_{k^2}$ has a row AND a column each with multiplicity at least $k-1$, as shown in Example 101 in [4, Table A].

1.6 Computer Programs and Examples

We have established some Matlab programs to facilitate the study of central digraphs. They are stored at:

```
http://www.resnet.wm.edu/~cklixx/matrixlib.html
```

The following programs can be found there:

1. MakeStandard(k)

   This program creates the standard matrix in $\mathcal{A}_{k^2}$.

2. MakeSwitch(p, q, r, s, A)

   This program performs the switch $[p, q; r, s]$ on a given $A \in \mathcal{A}_n$ as described in Section 3 if the switch is legal.

3. AllRanks(k)

   This program creates matrices in $\mathcal{A}_{k^2}$ of all possible ranks.

4. DRM(A)

   This program operates on a matrix $A \in \mathcal{A}_n$ and produces a permutationally similar matrix that exhibits "decreasing-row-multiplicity", i.e., rows with higher multiplicity are above rows with lower multiplicity and identical rows are adjacent. We present the following example of the transformation of the matrix $A \in A_9$ into $DRM(A)$:

$$A = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix}, \quad DRM(A) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

5. PerSim(A, B)

   This program checks whether two matrices $A, B \in \mathcal{A}_n$ are permutationally similar.

   In general, it is difficult to determine whether the zero-one matrices are permutationally similar. However, due to the special properties associated with the matrices in $\mathcal{A}_n$ (e.g.

constant row and column sums, sets of equal rows and columns, etc.) we are able to drastically reduce the number of necessary comparisons between matrices A and B that may or may not be similar. Preliminary tests such as verifying that the matrices have the same rank and have equal row and column multiplicity vectors are not sufficient to determine permutation similarity, but can be used initially in the program logic. The problem then reduces to actually performing all possible permutations on the matrices, a process that can be facilitated with special consideration of the row and column multiplicity vectors.

The computer program PerSim.m with the above considerations was implemented and utilized throughout our study of matrices A satisfying $A^2 = J$. Given two matrices A and B, preliminary testing was used to determine that the matrices have the same size, rank, multiplicity vectors, and that both in fact correspond to central groupoids. If the matrices were still possibly similar, then both were permuted into decreasing-row-multiplicity form and all possible permutations of the matrix A were considered. Under normal circumstances, a total of $n!$ permutations are necessary to exhaust all permutations of an $n \times n$ matrix. However, in decreasing-row-multiplicity form, one needs only to consider permutations within each set of equal rows and between sets of equal size. For example, given the matrix A above, we have a row multiplicity vector of $\{3, 2, 2, 1, 1\}$ and a column multiplicity vector of $\{3, 2, 2, 1, 1\}$. If a matrix B has the same multiplicity vectors, then one must only consider permutations within the three equal rows of A, within each of the two pairs of equal rows in A, and all further permutations after each possible swap of sets of rows of equal size. Consequently, the total number of permutations that need to be considered is $(3!)(2!)(2!)(2!)(2!) = 96$. When compared to $n! = 9! = 362880$ possible permutations, the program run-time has been considerably reduced. This allows us to finish the proof of Theorem 1.4.2.

Chapter 2

Solution Sets of Some Optimization Problems

2.1 Introduction

In this chapter, we study $m \times n$ $(0,1)-$matrices with the maximum number of 2×2 odd submatrices, i.e., submatrices with the sum of its entries equal to an odd integer, and several related problems. Like many other optimization problems in combinatorial matrix theory, it is often useful to convert a problem on $(0,1)-$matrices to a problem on $(-1,1)-$matrices. Obviously, one can convert a $(0,1)-$matrix to a $(-1,1)-$matrix by changing all the zero entries to -1. It is interesting that such a conversion can allow one to rephrase the objective function of the optimization problem in a more appealing analytic form, or reduce a given optimization problem to a simpler one or a problem of lower dimension; see [2] and our later discussion. For our first problem, one can easily rephrase it as:

Problem 1: Determine an $m \times n$ $(-1,1)-$matrix A such that A has the maximum number of 2×2 submatrices with nonzero determinant.

Here we observe that a 2×2 $(-1,1)-$matrix has an odd number of ones if and only if it has a nonzero determinant. We note that our study of this problem is related to certain factorial design problems in statistics; see [8].

Problem 2: Determine the maximum value of $\det(A^tA)$ over all $(-1,1)-$matrices A of size $m \times n$, assuming $m \geq n$.

As we will see, Problems 1 and 2 are closely related to the study of Hadamard matrices, a topic we shall address further later in our discussion.

While Problem 1 is quite well-studied in [11], we will present some different techniques to approach the problem including some computational approaches that advance the study of the remaining unsolved case, namely, $n \times n$ matrices with $n = 4k + 1$.

In Section 2, we present results relating Problems 1, 2, and Hadamard matrices via the unifying concept of compound matrices. In Section 3, we describe combinatorial techniques that can be used to study Problem 1. In Section 4, we present results for Problem 1 under the assumption that the Hadamard matrix conjecture is true, i.e. there always exists an $n \times n$ Hadamard matrix if $n = 4k$ for some integer $k > 0$. We will highlight matrices that attain the optimal values for Problems 1 and 2. Sections 5 and 6 are devoted to computational techniques we developed. In particular, a Tabu Search heuristic for the remaining unsolved case of Problem 1. Finally, in Section 7 we present suggestions for further research on these problems.

The following notations will be used in our discussion:

$\mathcal{A}_{m,n}(S), \mathcal{A}_n(S)$:	the set of $m \times n$ and $n \times n$ matrices, respectively, with entries in S, $S = \{0,1\}, \{-1,1\}$, or $\mathbf{R}$
$M^*_{m,n}(S), M^*_n(S)$:	the maximum number of odd matrices taken over the set $\mathcal{A}_{m,n}(S)$ and $\mathcal{A}_n(S)$, respectively, with $S = \{-1,1\}$ or $\{0,1\}$
$D^*_{m,n}(S), D^*_n(S)$:	the maximum determinant of matrices taken over the set $\mathcal{A}_{m,n}(S)$ and $\mathcal{A}_n(S)$, respectively, with $S = \{-1,1\}$ or $\{0,1\}$
$M(A)$:	the number of odd submatrices in A
$J_{m,n}$, J_n:	the matrix with entries all equal to 1 of size $m \times n$ and $n \times n$, respectively
$\mathrm{tr}\, A$:	trace of A, i.e., the sum of diagonal entries in A

2.2 Compound Matrices

Given an $m \times n$ matrix A and $k \leq \min\{m,n\}$, the kth compound matrix of A is the $\binom{m}{k} \times \binom{n}{k}$ matrix $C_k(A)$ whose entries are the determinants of the $k \times k$ submatrices of A arranged in lexicographical order. For example, if A is 3×4 and $d[i,j;k,l]$ denotes the determinant of the submatrix of A lying in rows i, j and columns k, l, then

$$C_2(A) = \begin{pmatrix} d[1,2;1,2] & d[1,2;1,3] & d[1,2;1,4] & d[1,2;2,3] & d[1,2;2,4] & d[1,2;3,4] \\ d[1,3;1,2] & d[1,3;1,3] & d[1,3;1,4] & d[1,3;2,3] & d[1,3;2,4] & d[1,3;3,4] \\ d[2,3;1,2] & d[2,3;1,3] & d[2,3;1,4] & d[2,3;2,3] & d[2,3;2,4] & d[2,3;3,4] \end{pmatrix}.$$

Clearly, Problem 1 reduces to asking for the matrix $A \in \mathcal{A}_{m,n}(\{-1,1\})$ with the maximum number of nonzero entries in $C_2(A)$. Since every odd submatrix in A gives rise to an entry of $C_2(A)$ with determinant ± 2, we see that the total number of nonzero entries in $C_2(A) = [\operatorname{tr} C_2(A)^t C_2(A)]/4$. By the properties of compound matrices, see [12], we have

$$\operatorname{tr} C_2(A)^t C_2(A) = \operatorname{tr} C_2(A^t A) = E_2(\lambda_1, \ldots, \lambda_n),$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of $A^t A$, and

$$E_2(x_1, \ldots, x_n) = \sum_{1 \le i < j \le n} x_i x_j$$

is the 2-elementary symmetric function. In other words, we have proved the following.

Theorem 2.2.1 *Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ denote the eigenvalues of an $n \times n$ matrix $A^t A$ where $A \in \mathcal{A}_n(\{-1,1\})$. Then,*

$$M(A) = \frac{1}{4} E_2(eig(A^t A)).$$

Therefore, the number of 2×2 odd submatrices in A can be calculated as a function of the eigenvalues of the matrix $A^t A$. We illustrate this result with the following example.

Example 2.2.2 Consider the matrix

$$B = \begin{pmatrix} + & + & + & + \\ + & + & - & - \\ + & - & + & + \\ - & + & - & - \end{pmatrix}.$$

Note that in matrix form, we represent every entry with value equal to 1 with a "+" and every entry with value equal to -1 with a "$-$". The eigenvalues of the matrix $B^t B$ are found to be $\lambda_1 = 0, \lambda_2 = 4, \lambda_3 = 6 + 2\sqrt{5}$, and $\lambda_4 = 6 - 2\sqrt{5}$. Consequently, we find:

$$\begin{aligned} M(B) &= \frac{1}{4} E_2(\lambda_1, \ldots, \lambda_4) \\ &= \frac{1}{4} E_2(0, 4, 6 + 2\sqrt{5}, 6 - 2\sqrt{5}) \\ &= \frac{1}{4} 24 + 8\sqrt{5} + 24 - 8\sqrt{5} + 36 - 12\sqrt{5} + 12\sqrt{5} - 20 \\ &= 16 \end{aligned}$$

Furthermore, note that Problem 2 can be rephrased as finding the maximum value of $\operatorname{tr} C_n(A^tA)$. In general, we have the following result.

Theorem 2.2.3 *Suppose S is the set of real matrices such that A^tA has diagonal entries all equal to n, $A \in S$, and A is $m \times n$ with $1 < m \leq n$. Then*

$$\max\{\operatorname{tr} C_k(A^tA) : A \in S\} \leq E_k(n, \ldots, n).$$

A matrix A satisfies the above as an equality if and only if $A^tA = nI_n$.

Proof. If we let

$$L(x_1, x_2, \ldots, x_m, \lambda) = f(x_1, x_2, \ldots, x_m) - \lambda(x_1 + x_2 + \cdots + x_m - m^2)$$

then we wish to maximize

$$f(x_1, x_2, \ldots, x_m) = \sum_{1 \leq i_1 < \cdots < i_k \leq m} x_{i_1} x_{i_2} \cdots x_{i_k}.$$

subject to

$$x_i \geq 0,\ x_1 + x_2 + \cdots + x_m = m^2.$$

We find:

$$\begin{aligned}
\frac{\partial L}{\partial x_1} &= \sum_{1 < j_1 < \cdots < j_{k-1} \leq m} x_{j_1} x_{j_2} \cdots x_{j_{k-1}} - \lambda = 0 \\
&\vdots \\
\frac{\partial L}{\partial x_t} &= \sum_{1 \leq j_1 < \cdots < t < \cdots < j_{k-1} \leq m} x_{j_1} x_{j_2} \cdots x_{j_{k-1}} - \lambda = 0 \\
&\vdots \\
\frac{\partial L}{\partial x_m} &= \sum_{1 \leq j_1 < \cdots < j_{k-1} < m} x_{j_1} x_{j_2} \cdots x_{j_{k-1}} - \lambda = 0
\end{aligned}$$

Now consider the subtraction $\frac{\partial L}{\partial x_a} - \frac{\partial L}{\partial x_b} = 0$. If we let $X_{\hat{a},\hat{b}} = \{x_1, \ldots, \hat{x_a}, \ldots, \hat{x_b}, \ldots, x_n\}$ denote the set of values x_1 to x_m not including x_a nor x_b, we find:

$$\frac{\partial L}{\partial x_a} - \frac{\partial L}{\partial x_b} = 0 \quad = \quad x_b E_{k-2}(X_{\hat{a},\hat{b}}) + E_{k-1}(X_{\hat{a},\hat{b}}) - \lambda$$
$$-x_a E_{k-2}(X_{\hat{a},\hat{b}}) - E_{k-1}(X_{\hat{a},\hat{b}}) + \lambda$$
$$= \quad (x_b - x_a) E_{k-2}(X_{\hat{a},\hat{b}})$$

Finally, since $E_{k-2}(X_{\hat{a},\hat{b}}) > 0$, we know that $x_a = x_b \ \forall (a,b)$ and $x_1 = x_2 = \cdots = x_m$. $\square$

In light of the above result, we now present the following definition.

Definition 2.2.4 *A matrix $A \in \mathcal{A}_n(\{-1,1\})$ satisfying $A^t A = nI_n$ is called a Hadamard matrix. In our discussion, we denote H_n as the set of all Hadamard matrices of order n.*

Consequently, by Theorem 2.2.3, ones sees immediately that if A is an $m \times n$ submatrix of a Hadamard matrix, then it will be optimal for Problems 1 and 2.

2.3 Combinatorial Techniques

A simple yet powerful observation is that $M^*_{m,n}(\{0,1\}) = M^*_{m,n}(\{-1,1\})$ for all pairs of values (m,n). In other words, given the $m \times n$ matrix A where $M(A) = M^*_{m,n}(\{0,1\})$, create the matrix B equal to $2A - J_{m,n}$ and note that $M(B) = M^*_{m,n}(\{-1,1\})$. Thus, B attains the maximum possible number of 2×2 submatrices with an odd number of 1's. To this effect, in our combinatorial analysis we consider only $(-1,1)-$matrices.

As seen in [11], the derivations of matrices B satisfying $M(B) = M^*_{m,n}(\{-1,1\})$ for $m < n$ usually involve relatively simple manipulations of the matrix A satisfying $M(A) = M^*_n(\{-1,1\})$. For example, as we shall see later in our discussion, the matrix $A_{7,8}$ that attains $M(A_{7,8}) = M^*_{m,n}(\{-1,1\})$ can be created by removing any of the rows of the matrix $A_{8,8}$ attaining $M(A_{8,8}) = M^*_{8,8}(\{-1,1\})$. As a result, we shall narrow our search to consider only square matrices, i.e. $A \in \mathcal{A}_n(\{-1,1\})$. We propose that the remaining cases, where $m < n$, are considerably less difficult once the true value of $M^*_n(\{-1,1\})$ is known. Finally, we shall simplify our notation so as to drop consideration of the cases where $S = \{0,1\}$ or $\mathbf{R}$. In other words, from this point on we let $\mathcal{A}_n$ denote $\mathcal{A}_n(\{-1,1\})$, M^*_n denote $M^*_n(\{-1,1\})$, and D^*_n denote $D^*_n(\{-1,1\})$.

The following counting method is exactly the one used in [11].

Theorem 2.3.1 *Let $k^+_{i,j}$ denote the number of positions in rows (columns) i and j such that the two rows (columns) agree, i.e. both have entries equal to 1 or -1. Similarly, let $k^-_{i,j}$ denote the number of positions in rows (columns) i and j such that the two disagree. Then, the number of odd submatrices over rows (columns) i and j can be determined by $k^+_{i,j} * k^-_{i,j}$.*

Proof. Without loss of generality, assume that rows i and j have the following form:

$$\begin{pmatrix} + & \dots & + & + & \dots & + \\ + & \dots & + & - & \dots & - \end{pmatrix}$$

In other words, there are $k^+_{i,j}$ columns of the form $(+ \quad +)^t$ (form S) and $k^-_{i,j}$ columns of the form $(+ \quad -)^t$ (form D). Over the entire pair of rows, there are exactly $\binom{n}{2}$ submatrices. In order for a submatrix to be odd, one row must have the form S and the other must have form D. Consequently, the number of odd submatrices over rows i and j is equal to $k^+_{i,j} * k^-_{i,j}$. To see that the same conditions hold for columns i and j, consider the transpose of the two columns. □

As illustrated by the above theorem, the number of odd submatrices over an entire matrix $A \in \mathcal{A}_n$ can be counted in a straightforward manner. Since every 2×2 submatrix in A can be defined as some member of a pair of two rows in A, the total number of odd submatrices in A can be found by:

$$M(A) \quad = \sum_{1 \le i < j \le n} k^+_{i,j} * k^-_{i,j}. \qquad (2.3.1)$$

As an illustration of this technique, consider the following example.

Example 2.3.2 Return to the matrix B given in Example 2.2.2. By Equation 2.3.1, we count the total number of odd submatrices by

$$\begin{aligned} M(B) &= \sum_{1 \le i < j \le 4} k^+_{i,j} * k^-_{i,j} \\ &= k^+_{1,2} * k^-_{1,2} + k^+_{1,3} * k^-_{1,3} + k^+_{1,4} * k^-_{1,4} + k^+_{2,3} * k^-_{2,3} + k^+_{2,4} * k^-_{2,4} + k^+_{3,4} * k^-_{3,4} \\ &= 2 * 2 + 3 * 1 + 1 * 3 + 1 * 3 + 3 * 1 + 0 * 4 \\ &= 16 \end{aligned}$$

Before considering the problem of finding a matrix A satisfying $M(A) = M_n^*$ for individual values of n, we establish generous upper and lower bounds of $M(A)$ for any size. Note that for the matrix J_n, with a 1 in every position, there are exactly zero odd submatrices. Therefore, $M(A) \geq 0$ for all A, where equality holds if and only if A is equal to J_n. Furthermore, for even n, we find that the maximum number of odd submatrices within any pair of rows or columns is found if and only if $k_{i,j}^+ = k_{i,j}^- = \frac{n}{2}$. In this case, we say that each pair of rows is a "perfect" pair, see [11]. Similarly, for odd n, we find that the maximum number of odd submatrices within any pair of rows or columns is found if and only if $k_{i,j}^+ = \frac{n+1}{2}$ and $k_{i,j}^- = \frac{n-1}{2}$, or vice versa. In this case, we say that each pair of rows is a "nearly-perfect" pair, see [11]. If there exists some matrix $A_p \in \mathcal{A}_n$ with the property that all pairs of rows are "perfect" ("nearly-perfect") for n even (odd), then $M(A_p) = M_n^*$ and the following bounds can be established for all $A \in \mathcal{A}_n$.

$$\text{n is even} \quad \Rightarrow \quad 0 \leq M(A) \leq \left(\frac{n}{2}\right)^2 \binom{n}{2} \tag{2.3.2}$$

$$\text{n is odd} \quad \Rightarrow \quad 0 \leq M(A) \leq \frac{n-1}{2}\frac{n+1}{2}\binom{n}{2} \tag{2.3.3}$$

Here we also note that the value of $k_{i,j}^+ * k_{i,j}^-$ is directly related to the inner product of rows i and j. In fact, if we let a_i and a_j denote the ith and jth rows of A, respectively, then $k_{i,j}^+ - k_{i,j}^- = a_i \cdot a_j$. Consequently, we have the following theorem.

Theorem 2.3.3 *If the inner product of all pairs of rows in the matrix A is equal to 0, then A is "perfect". Furthermore, if the inner product of all pairs of rows in the matrix B is equal to ± 1, then B is "nearly-perfect". The inner product of row i and row j in A is found as the (i, j) entry in the matrix $A^t A$.*

Proof: The proof is straightforward.

As expected, there may exist many matrices $A^{(1)}, A^{(2)}, \ldots, A^{(k)}$ such that $M(A^{(1)}) = M(A^{(2)}) = \cdots = M(A^{(k)})$ for some integer k. In fact, given a matrix $A \in \mathcal{A}_n$, a variety of operations can be performed on A to produce a matrix A' such that $M(A) = M(A')$, see [11]. We provide proofs of these instances for the sake of completeness.

Theorem 2.3.4 *Given a matrix $A \in \mathcal{A}_n$, the matrix A' obtained by any combination of the following operations satisfies $M(A) = M(A')$.*

1. *Let A' equal A^t.*

2. Permute any pairs of rows or any pairs of columns.

3. Multiply any row or column by -1.

Proof: For both (1) and (2), the fact that these operations do not change the total number of odd submatrices is clear. After either operation, the collection of unordered rows (or columns) is equal for A and A', so $M(A)$ is certainly equal to $M(A')$. Finally, for (3), let i denote the index of the row in A that has been altered. The total number of odd submatrices over all pairs of rows j and k where $j \neq i$ and $k \neq i$ is certainly equal for A and A'. Now, consider all pairs of rows i and j. Any positions in rows i and j that agree in A must disagree in A'. Similarly, any positions that disagree in A must agree in A'. Consequently, over all pairs of rows i and j, we have $k^+_{i,j}(A) * k^-_{i,j}(A) = a * b = k^-_{i,j}(A') * k^+_{i,j}(A')$, which implies $M(A) = M(A')$.

2.4 Optimal Solutions

In the following discussion, we study the optimal solutions of Problem 1 based on the assumption that the Hadamard Conjecture is valid. As we shall find, this problem can be split naturally into four distinct cases based on the value of n. For the first three cases, previous proofs of optimum values exist and are described along with some alternative approaches that have been considered. The final case, however, remains open for large n.

2.4.1 $n = 4k$ and Hadamard Matrices

Begin by returning to Definition 2.2.4 given previously. Research on Hadamard matrices is rich and extensive, and despite the lack of a proof of their existence for all values of $n = 4k$, libraries of examples have been found for many values of n. For simplicity, we assume throughout our study that a Hadamard matrix exists for all desired values of $n = 4k$. Given that $A \in H_n$ exists, it is well known that the eigenvalues of A^tA are $\{n, n, \ldots, n\}$. Therefore, by Theorem 2.2.3 we find that $A \in H_n$ attains $M(A) = M^*_n$ and $\det(A) = D^*_n$. Furthermore, since all pairs of rows i and j such that $i \neq j$ have an inner product of 0, a Hadamard matrix is described as "perfect".

Based on the structure of Hadamard matrices, one of the methods used during this study was the manipulation of Hadamard matrices to find matrices A satisfying $M(A) = M^*_n$ for values of $n \neq 4k$ for some integer k. For example, given $A \in H_n$, consider the $(n-1) \times (n-1)$ matrix B found by the removal of one row and one column from A. How does $M(B)$ relate to M^*_{n-1}? Furthermore, how does the removal of two or three rows and columns from A

relate to M^*_{n-2} and M^*_{n-3}, respectively? Rather than the removal of a row and column from a Hadamard Matrix, is there a straightforward way to add a row and a column to A to form a $(n+1) \times (n+1)$ matrix C that satisfies $M(C) = M^*_{n+1}$? We consider these techniques for the remaining cases.

2.4.2 $n = 4k - 1$

The optimum value M^*_n for each n in this case has been established prior to our study, see [11]. However, we present an alternative proof based on compound matrix theory.

Theorem 2.4.1 *Given the $(n+1) \times (n+1)$ matrix A is Hadamard, the matrix formed by the removal of any row and any column from A is a matrix B having a total of*

$$M(B) = \frac{n-1}{2}\frac{n+1}{2}\binom{n}{2}$$

odd submatrices. Furthermore, B attains the maximum possible number of odd submatrices over all $(-1,1)-$matrices of order n, i.e. B is "nearly-perfect" and $M(B) = M^*_n$.

Proof: Consider the Hadamard matrix A with $eig(A^tA) = \{n+1, n+1, \ldots, n+1\}$. We wish to remove row i and columns j. According to the conditions of Theorem 2.3.4, perform the necessary operations to assure that column j has all entries equal to 1. Upon removal of row i and column j, we are left with the matrix B. Furthermore, the following equality holds:

$$B^tB = (n+1)I_n - J_n$$

The eigenvalues of the first term and of the second term are given by the sets G_1 and G_2, respectively, where

$$G_1 = \{\underbrace{n+1, \ldots, n+1}_{n}\} \text{ and } G_2 = \{n, \underbrace{0, \ldots, 0}_{n-1}\}.$$

Consequently,

$$eig(B^tB) = eig((n+1)I_n - J_n) = \{1, \underbrace{n+1, \ldots, n+1}_{n-1}\}$$

The corresponding counting method based on Theorem 2.2.1 yields:

$$M(B) \quad = \quad \frac{1}{4}E_2(\lambda(B^tB))$$

$$= \frac{1}{4}\left((n-1)(n+1) + \binom{n-1}{2}(n+1)^2\right)$$
$$= \frac{n-1}{2}\frac{n+1}{2}\binom{n}{2}$$

so many odd submatrices in the resulting matrix. □

Under the pair-wise consideration of rows counting method, we also determine the total number of odd submatrices by noting that the removal of one column and one row from the matrix H_{n+1} results in a matrix with "nearly-perfect" pairs of rows i, j for all $1 \leq i < j \leq n$.

Unfortuntely, the value of D_n^* is unknown for many values of $n = 4k-1$. In fact, the only known cases are $n = 3, 7$, and 11, see [8]. Of these only the matrix attaining $\det(A) = D_3^*$ satisfies $M(A) = M_n^*$. Consequently, there seems to be no connection between the matrices attaining optimal values for Problems 1 and 2 in this case.

2.4.3 $n = 4k - 2$

Similar to the $n = 4k-1$ case, a proof of the optimum value of M_n^* for $n = 4k-2$ previously exists, see [11]. However, we shall again present a similar construction technique based on the manipulation of Hadamard matrices.

Theorem 2.4.2 *Given $A \in H_{n+2}$ is Hadamard, then a matrix B of order n formed by the removal of two rows and two columns from H_{n+2} has a maximum of*

$$M(B) = \frac{1}{8}n^4 - \frac{1}{8}n^3 - \frac{1}{4}n^2 + \frac{n}{2}$$

odd submatrices.

Proof: Let a_i and a_j represent the ith and jth columns of the matrix A, respectively. Without loss of generality we may assume

$$a_i = (\underbrace{+ \ \cdots \ +}_{n+2})^t \text{ and } a_j = (\underbrace{+ \ \cdots \ +}_{\frac{n+2}{2}} \ \underbrace{- \ \cdots \ -}_{\frac{n+2}{2}})^t.$$

There are two cases: (1) remove one row from rows 1 through $\frac{n+2}{2}$ and one row from rows $\frac{n+2}{2} + 1$ through $n + 2$, or (2) remove two rows from the top half of the matrix or two rows from the bottom half.

Case 1: Upon removal of the two rows in the matrix A, we are left with the matrix B' with all rows mutually orthogonal to each other, i.e. they have inner product equal to 0. Let

x be the ith column and y be the jth column of B', respectively, then the following equality holds:

$$B^tB + x^tx + y^ty = (n+2)I_n$$

Solving for the product B^tB, we find the following result.

$$\begin{aligned} B^tB &= (n+2)I_n - J_n - (\underbrace{+ \cdots +}_{\frac{n+2}{2}-1} \underbrace{- \cdots -}_{\frac{n+2}{2}-1})^t(\underbrace{+ \cdots +}_{\frac{n+2}{2}-1} \underbrace{- \cdots -}_{\frac{n+2}{2}-1}) \\ &= (n+2)I_n - J_n - \begin{pmatrix} J_{\frac{n+2}{2}-1} & -J_{\frac{n+2}{2}-1} \\ -J_{\frac{n+2}{2}-1} & J_{\frac{n+2}{2}-1} \end{pmatrix} \\ &= \begin{pmatrix} (n+2)I_{\frac{n}{2}} & 0 \\ 0 & (n+2)I_{\frac{n}{2}} \end{pmatrix} - \begin{pmatrix} 2J_{\frac{n+2}{2}-1} & 0 \\ 0 & 2J_{\frac{n+2}{2}-1} \end{pmatrix} \end{aligned}$$

Finally, in the result above, the eigenvalues of the first term, the second term, and of the entire expression are found to be G_1, G_2, and G_3, respectively, where

$$G_1 = \{\underbrace{n+2, \ldots, n+2}_{n}\},\ G_2 = \{n, n, \underbrace{0, \ldots, 0}_{n-2}\},\ \text{and } G_3 = \{2, 2, \underbrace{n+2, \ldots, n+2}_{n-2}\}.$$

Case 2: Without loss of generality, assume that two rows are removed from the top half of the matrix A. Now, similar to the above, if we let x be the ith column and y be the jth column of the matrix C' formed by the removal of these two rows, then the following equation holds:

$$C^tC + x^tx + y^ty = (n+2)I_n$$

In the same manner as before, solving for the product C^tC yields:

$$C^tC = \begin{pmatrix} (n+2)I_{\frac{n+2}{2}-2} & 0 \\ 0 & (n+2)I_{\frac{n+2}{2}} \end{pmatrix} - \begin{pmatrix} 2J_{\frac{n+2}{2}-2} & 0 \\ 0 & 2J_{\frac{n+2}{2}} \end{pmatrix}$$

The eigenvalues of the first term, the second term, and of the entire expression are found to be G_4, G_5, and G_6, respectively, where

$$G_4 = \{\underbrace{n+2, \ldots, n+2}_{n}\},\ G_5 = \{n+2, n-2, \underbrace{0, \ldots, 0}_{n-2}\},\ \text{and } G_6 = \{0, 4, \underbrace{n+2, \ldots, n+2}_{n-2}\}.$$

Counting the number of odd submatrices of the matrices resulting from the two cases, we find

$$M(B) = \frac{1}{4}E_2(2, 2, n+2, \ldots, n+2) = \frac{1}{4}(4 + \binom{(n-2)}{2}(n+2)^2 + \binom{2}{1}\binom{n-2}{1}2(n+2))$$

$$M(C) = \frac{1}{4}E_2(0,4,n+2,\ldots,n+2) = \frac{1}{4}(\binom{(n-2)}{2}(n+2)^2 + \binom{2}{1}\binom{n-2}{1}2(n+2)).$$

Therefore, considering the procedure described in case 1, we have found that a matrix B formed by the removal of two rows and two columns from a Hadamard matrix A has a maximum of $M(B) = \frac{1}{8}n^4 - \frac{1}{8}n^3 - \frac{1}{4}n^2 + \frac{n}{2}$ odd submatrices. □

In fact, when compared to the previously proven value of M_n^*, the above approach attains the maximum number of odd submatrices. We mention the following result with proof given in [11].

Theorem 2.4.3 *Let $A \in \mathcal{A}_n$ where $n = 4k-2$. The maximum number of odd 2×2 submatrices occurs when the rows of A are split into two sets of equal size such that rows i and j have $a_i \cdot a_j = 0$ if i and j are in the different sets and $a_i \cdot a_j = \pm 2$ if i and j are in the same set.*

One can easily see that the resulting matrix B from Theorem 2.4.2 has these characteristics. Therefore, $M(B) = M_n^*$.

When matrices of this type are compared to those attaining $\det(A) = D^*(A)$, we find an interesting connection between our two problems. According to [8], a matrix A is known to satisfy $\det(A) = D_n^*$ if

$$A^tA = \begin{pmatrix} B & 0 \\ 0 & B \end{pmatrix}$$

where $B = (n-2)I_m + 2J_m$, $m = \frac{n}{2}$. Furthermore, such matrices, defined as *Ehlich−Wojtas*-type matrices, are known to exist only if $2(n-1)$ is the sum of two perfect squares. In other words, for the cases where these matrices exist, one can easily see that A being of *Ehlich−Wojtas*-type satisfies $\det(A) = D_n^*$ and $M(A) = M_n^*$. However, for ALL $n = 4k-2$, matrices formed by Theorem 2.4.2 are known to NOT satisfy $\det(A) = D_n^*$, i.e. they cannot be expressed as *Ehlich − Wojtas*-type matrices. Thus, the solution set of Problem 2 is a proper subset of that of Problem 1.

2.4.4 $n = 4k + 1$

In this section we discuss perhaps the most difficult case of this problem. Preliminary bounds have been established, see [11], and we provide a similar proof for the sake of completeness. However, true values of M_n^* appear to be known only for small cases, i.e. $n = 5, 9, 13$. For each known case we present proofs of optimality along with a presentation of techniques that may be applied to larger cases. In the following two sections, we present computational methods for lower dimensions.

Theorem 2.4.4 *If a matrix A of order $n-1$ is Hadamard, then there exists a matrix B of order $n = 4k+1$ satisfying $M(B) = 32k^4 + 24k^3 + 6k - 2$. Consequently, for any $n = 4k+1$ the value M_n^* is bounded in the following manner.*

$$32k^2 + 24k^3 + 6k - 2 \leq M_{4k+1}^* \leq 32k^4 + 24k^3 + 4k^2$$

Proof: Under the conditions of Theorem 2.3.4, perform the necessary series of operations on the matrix A to form the matrix A' with all entries equal to 1 along the first row and column. Furthermore, let b be the $1 \times (n-1)$ vector with all entries equal to -1 except the first position which is equal to 1. That is,

$$b = (+ \underbrace{- \;\cdots\; -}_{n-2}).$$

Now, consider the following augmented matrix B.

$$B = \begin{pmatrix} A' & b^t \\ b & 1 \end{pmatrix}$$

The number of odd submatrices in B is counted in the following manner. First, note that each pair of rows i and j, $i < j$, within the first $n-1$ rows of B are "nearly-perfect" pairs with inner product equal to -1 if $i = 1$ and inner product equal to 1 otherwise. Second, let $j = n$ and consider the possible pairs of rows (i, j) with $1 \leq i \leq (n-1)$. For $2 \leq i \leq (n-1)$, the rows i and j represent "nearly-perfect" pairs while for $i = 1$ the rows agree in only the first and last positions. In other words, there are $2(4k-1)$ odd submatrices in the first and last rows. Thus, the value M_{4k+1}^* is bounded below by

$$M(B) = (\binom{4k+1}{2} - 1)(2k)(2k+1) + 2(4k-1) = 32k^4 + 24k^3 + 6k - 2 \leq M_{4k+1}^*$$

and above by

$$M_{4k+1}^* \leq \frac{4k}{2}\frac{4k+2}{2}\binom{4k+1}{2} = 32k^4 + 24k^3 + 4k^2.$$

□

Although the above bounds are guaranteed to hold for all $n = 4k+1$, the difference between the two bounds is significant for large n. Therefore, do alternative methods exist that could improve the bounds given above? Is there a certain subset of $n = 4k+1$ that can be proven to attain a certain value of M_n^*? As a consideration of these questions, we begin again with the technique of removing rows and columns from a matrix $A \in H_{n+3}$, i.e. A is Hadamard.

Theorem 2.4.5 *Given $A \in H_{n+3}$ is Hadamard and $n \geq 5$, then a matrix B with order n formed by the removal of three rows and three columns from A attains a maximum of*

$$M(B) = \frac{1}{8}n^4 - \frac{1}{8}n^3 - \frac{3}{8}n^2 + \frac{9}{8}n - \frac{3}{4}$$

odd submatrices.

Proof: Similar to the procedures used for $n = (4k-1)$ and $n = (4k-2)$, we find that the removal of three rows and three columns is far more challenging. Let a_x, a_y, and a_z represent the xth, yth, and zth columns of A, respectively. Without loss of generality we may assume

$$a_x = (\underbrace{+ \cdots +}_{n+3})^t, \; a_y = (\underbrace{+ \cdots +}_{\frac{n+3}{2}} \; \underbrace{- \cdots -}_{\frac{n+3}{2}})^t,$$

$$\text{and } a_z = (\underbrace{+ \cdots +}_{\frac{n+3}{4}} \; \underbrace{- \cdots -}_{\frac{n+3}{4}} \; \underbrace{+ \cdots +}_{\frac{n+3}{4}} \; \underbrace{- \cdots -}_{\frac{n+3}{4}}).$$

To illustrate this procedure, we consider the removal of one row from the top quarter, one from the second quarter, and one from the third quarter of A. This scheme will lead to the maximum number of odd submatrices that can be achieved through this method. In fact, the indices of the three rows that are to be removed can each come from any of the distinct quarters of A defined by the unique rows of the submatrix $[a_x \; a_y \; a_z]$. However, we leave consideration of the remaining cases to the interested reader. For the given case, let b_x, b_y, and b_z represent the xth, yth, and zth column of the matrix B' formed by the removal of the specified rows. Thus, the following equation

$$B^tB + b_x^tb_x + b_y^tb_y + b_z^tb_z = (n+3)I_n$$

holds and we solve for B^tB to find

$$\begin{aligned} B^tB &= (n+3)I_n - b_x^tb_x - b_y^tb_y - b_z^tb_z \\ &= (n+3)I_n - J_n - P^t \begin{pmatrix} 2J_{\frac{n+3}{4}-1} & -2J_{\frac{n+3}{4}-1} & 0 & 0 \\ -2J_{\frac{n+3}{4}-1} & 2J_{\frac{n+3}{4}-1} & 0 & 0 \\ 0 & 0 & 2J_{\frac{n+3}{4}-1} & -2J_{\frac{n+3}{4}-1,\frac{n+3}{4}} \\ 0 & 0 & -2J_{\frac{n+3}{4}-1,\frac{n+3}{4}} & 2J_{\frac{n+3}{4}} \end{pmatrix} P \end{aligned}$$

$$= P^t \left((n+3)I_n - J_n - \begin{pmatrix} 2J_{\frac{n+3}{4}-1} & -2J_{\frac{n+3}{4}-1} & 0 & 0 \\ -2J_{\frac{n+3}{4}-1} & 2J_{\frac{n+3}{4}-1} & 0 & 0 \\ 0 & 0 & 2J_{\frac{n+3}{4}-1} & -2J_{\frac{n+3}{4}-1,\frac{n+3}{4}} \\ 0 & 0 & -2J_{\frac{n+3}{4}-1,\frac{n+3}{4}} & 2J_{\frac{n+3}{4}} \end{pmatrix} \right) P$$

where P is a permutation matrix with entries in $\{0,1\}$. The eigenvalues of the above expression are found to be

$$G = \{1, 4, 4, \underbrace{n+3, \ldots, n+3}_{n-3}\}$$

Consequently,

$$\begin{aligned} M(B) &= \frac{1}{4}(2(4) + (n+3)(n-3) + 4(4) + 2(4(n+3))(n-3) + (n+3)^2\binom{n-3}{2}) \\ &= \frac{1}{8}((n+3)^4 - 13(n+3)^3 + 60(n+3)^2 - 108(n+3) + 48) \\ &= \frac{1}{8}n^4 - \frac{1}{8}n^3 - \frac{3}{8}n^2 + \frac{9}{8}n - \frac{3}{4}. \end{aligned}$$

□

Unfortunately, when compared to the bound given in Theorem 2.4.4, the above bound fails to compete. In other words, consider the lower bound of Theorem 2.4.4, call it $M(L)$, and the maximum number of odd submatrices that can be formed by the procedure in Theorem 2.4.5, call it $M(U)$. After expanding each in terms of the common variable k, i.e. $n = 4k+1 \Rightarrow k = \frac{n-1}{4}$, we are left with the inequality

$$M(U) = 32k^4 + 24k^3 + 2k < 32k^4 + 24k^3 + 6k - 2 = M(L)$$

for $k \geq 1$. Although other techniques may exist for the manipulation of larger Hadamard matrices to create matrices with order $n = 4k+1$ that attain $M(A) = M_n^*$, the above suggests that a more lucrative search technique is the augmentation of smaller Hadamard matrices rather than the reduction of larger ones. To this effect, consider the following proposition.

Proposition 2.4.6 *If $A \in \mathcal{A}_n$ satisfies $M(A) = M_n^*$ and $n = 4k+1$ for some positive integer k, then there exists a submatrix B of A with order $n-1$ having $B \in H_{n-1}$.*

A proof of this proposition would suggest that there may exist a clever "padding" method that could always augment a Hadamard matrix of order $n-1$ with one row and one column to produce a matrix A satisfying $M(A) = M_n^*$. Unfortunately, the difficultly in this case is further illustrated in the fact that a counterexample to this proposition exists for $n = 13$ (see the subsequent section on the 13×13 case below). Regardless, alternative "padding" methods similar to the one provided in Theorem 2.4.4 may produce better bounds on the value of M_n^*.

Proposition 2.4.7 *A lower bound on the value of M_{4k+1}^* may be produced by total enumeration of the possible rows and columns with entries in $\{-1, 1\}$ that can be added to a matrix $A \in H_{4k}$. With two possible entries in each position, there are 2^{8k+1} possible combinations of rows and columns.*

The program `pad_Hadamard_search.m` was developed to consider this approach for small values of $n = 4k + 1$. As expected, however, the program is highly inefficient for large values of n and the run-time is extremely long.

At this point, we begin consideration of $n = 4k + 1$ for $n = 5, 9$, and 13. A variety of techniques are presented along with proofs for the value of M_n^* for these small cases.

5×5 case

Consider the matrix A_5 in Appendix A obtained by total enumeration of possible rows and columns with entries in $\{-1, 1\}$ that could be used to "pad" a 4×4 Hadamard submatrix. A_5 represents the "best" matrix found by this procedure, i.e. $M(A_5) = \binom{5}{2}(3 * 2)$ and by Equation 2.3.3, $M(A_5) = M_5^*$.

The important structure of A_5 is revealed when considering the matrix $A_5^t A_5$, namely the 5×5 matrix with 5's along the main diagonal and 1's in all off-diagonal entries. According to Theorem 2.3.3, A_5^* is "nearly-perfect". Do other values of $n = 4k + 1$ exist such that a matrix with the above characteristics can be formed? Consider the following theorem, see [8].

Theorem 2.4.8 *A matrix $A \in \mathcal{A}_n$ satisfying*

$$A^t A = \begin{pmatrix} n & \pm 1 & \cdots & \pm 1 \\ \pm 1 & n & \ddots & \vdots \\ \vdots & \ddots & \ddots & \pm 1 \\ \pm 1 & \cdots & \pm 1 & n \end{pmatrix}$$

exists only if $2n - 1 = 2(4k + 1) - 1 = 8k + 1$ is the square of an integer.

Proof: Let $|X|$ denote the determinant of the matrix X. Then,

$$|A| = \sqrt{|A^tA|} = \sqrt{|(n-1)I_n + J_n|} = \sqrt{(n-1)^{n-1}(2n-1)} = (4k)^{2k}\sqrt{2n-1}.$$

Finally, the determinant of A must be an integer, which implies $2n-1$ is the square of some integer. □

As a result of Theorem 2.4.8, we know that a matrix of order $n = 4k+1$ can have inner product structure similar to A_5 only if $2n-1$ is the square of some integer. We stress, however, that this condition is necessary, but not sufficient. A matrix A of this type will be defined to be an *Ehlich*-type matrix to follow the notation of [8]. Note that A will then always be "nearly-perfect" and thus attains $M(A) = M_n^*$. Furthermore, also by [8], we note that if an *Ehlich*-type matrix A exists for a given value of n, then $\det(A) = D_n^*$. Thus, $\det(A_5) = D_n^*$.

9×9 case

By Theorem 2.4.8, a *Ehlich*-type matrix does not exist for $n = 9$. As a result, we discuss a proof by the lack of a counterexample to solve this case.

Consider the bounding technique in Theorem 2.4.4. The matrix A_9 (see Appendix A) formed by this procedure has $M(A_9) = 714$ while the maximum number of odd submatrices can be bounded by $714 \leq M_n^* \leq 720$. Does there exist a matrix $A \in \mathcal{A}_n$ with $M(A) > M(A_9)$? If so, what inner product structures could the matrix A have?

In order to show that $M(A_9) = M_9^*$, we must show:

(1) No matrix $A \in \mathcal{A}_9$ has every pair of rows with inner product equal to ± 1. In this case, $M(A) = \binom{9}{2}(5 * 4) = 720 = M_9^*$.

(2) There does not exist a matrix $A \in \mathcal{A}_9$ such that exactly k pairs of rows, $1 \leq k \leq 2$, have an inner product of ± 3 while the remaining pairs have inner product equal to ± 1. Such a matrix would have $M(A) = (\binom{9}{2} - 1) + 18 = 718$ for $k = 1$ or $M(A) = (\binom{9}{2} - 2) + 2(18) = 716$ for $k = 2$. We are not interested in $k > 2$ since this would yield $M(A) \leq 714$, the number of odd submatrices already found in A_9.

Of course, (1) would imply that a *Ehlich*-type matrix exists for $n = 9$, which we already know to be impossible. Therefore, the search is reduced to (2). If a matrix exists that would satisfy the elements of (2), how may such a matrix be constructed? We propose the following construction technique.

Up to permutation similarity, we wish to determine as many rows of the 9×9 matrix A that have inner product equal to ± 1 as possible. If A is to satisfy $M(A) > M(A_9)$, then we propose at least $n - 2 = 7$ rows must have this property. Otherwise, there would be at least $k = 3$ pairs of rows with inner product $p \leq -3$ or $p \geq 3$. If we let $A = \begin{pmatrix} a_1 & a_2 & \dots & a_9 \end{pmatrix}^t$, then by Theorem 2.3.4 we may assume

$$a_1 = (\underbrace{+ \ \dots \ +}_{9})$$

and that $a_1 \cdot a_i = 1 \ \forall \ i \geq 2$, or else multiply row a_i by -1. Furthermore, assume

$$a_2 = (\underbrace{+ \ \dots \ +}_{5} \ \underbrace{- \ \dots \ -}_{4})$$

so $a_2 \cdot a_j = \pm 1 \ \forall \ j \geq 3$. Consider a_j with $3 \leq j \leq 9$. We know that $a_1 \cdot a_j = 1$, which implies that row j has four -1's and five 1's, at least one of which appears in the first five columns of A. Let k denote the number of 1's in a_j positioned in the first five columns of A. Consequently, there are $5 - k$ -1's in the first five columns, $5 - k$ 1's in the last four columns, and $4 - (5 - k)$ -1's in the last four columns. This set of parameters implies that the following diophantine equation must hold.

$$\begin{aligned} \pm 1 &= a_2 \cdot a_j \\ &= k - (5 - k) - (5 - k) + (4 - (5 - k)) \\ &= 4k - 11 \end{aligned}$$

Since k must be an integer, $a_2 \cdot a_j = 1$ and $k = 3$ for all $j \geq 3$. Up to permutation similarity, A must have

$$(a_1 \ a_2 \ a_3)^t = \begin{pmatrix} + & + & + & + & + & + & + & + & + \\ + & + & + & + & + & - & - & - & - \\ + & + & + & - & - & + & + & - & - \end{pmatrix}.$$

Although the above procedure is somewhat tedious when considering the remaining rows, the ability to theoretically determine as many rows of the matrix A as possible is extremely advantageous when considering many computational techniques. More specifically, any predetermined structure in A will drastically decrease the number of conditions that must be tested in a computer experiment.

With respect to the search for a matrix A that satisfies $M(A) > M(A_9)$, we propose that A may be constructed by the sequential addition of rows 4 through 9 that yield a predetermined number of odd submatrices after each addition. In other words, when considering the addition of row i to the matrix $(\,a_1 \quad a_2 \quad \ldots \quad a_{i-1}\,)^t$, we may rule out all row additions that would yield a matrix $(\,a_1 \quad a_2 \quad \ldots \quad a_i\,)^t$ that would not be able to attain $M(A) > M(A_9)$ after the addition of rows a_{i+1} through a_9 based on $M((\,a_1 \quad a_2 \quad \ldots \quad a_i\,)^t)$.

For $n = 9$, this procedure is not a hard one. In general, however, if A_b is the "best" matrix yet found for a given value of n, then the following table illustrates the difficulties in enumerating all possible sets of inner products of the rows of a matrix A that will provide $M(A) > M(A_b)$. Let $K(A)$ denote the set of inner products of all pairs of rows i and j, $i < j$, in the matrix A. Therefore, $|K| = \binom{n}{2}$. Furthermore, let $K'(A)$ equal the set of the absolute values of all entries in $K(A)$ not equal to 1. For example, if $K(A) = \{1, 1, -1, -1, 3, -5\}$, then $K'(A) = \{3, 5\}$. Finally, let $(a)^b$ represent the entry a having multiplicity of b and let

$$N_1 = \frac{n+1}{2}\frac{n-1}{2}, N_3 = \frac{n+3}{2}\frac{n-3}{2}.$$

Table 2.4.1

$K'(A)$					$M(A)$
$\{\}$					$(\binom{n}{2})N_1$
$\{3\}$					$(\binom{n}{2} - 1)N_1 + N_3$
$\{(3)^2\}$					$(\binom{n}{2} - 2)N_1 + 2N_3$
$\{(3)^3\}$	$\{5\}$				$(\binom{n}{2} - 3)N_1 + 3N_3$
$\{(3)^4\}$	$\{5, 3\}$				$(\binom{n}{2} - 4)N_1 + 4N_3$
$\{(3)^5\}$	$\{5, (3)^2\}$				$(\binom{n}{2} - 5)N_1 + 5N_3$
$\{(3)^6\}$	$\{5, (3)^3\}$	$\{(5)^2\}$		$\{7\}$	$(\binom{n}{2} - 6)N_1 + 6N_3$
$\{(3)^7\}$	$\{5, (3)^4\}$	$\{(5)^2, 3\}$		$\{7, 3\}$	$(\binom{n}{2} - 7)N_1 + 7N_3$
$\{(3)^8\}$	$\{5, (3)^5\}$	$\{(5)^2, (3)^2\}$		$\{7, (3)^2\}$	$(\binom{n}{2} - 8)N_1 + 8N_3$
$\{(3)^9\}$	$\{5, (3)^6\}$	$\{(5)^2, (3)^3\}$	$\{(5)^3\}$	$\{7, (3)^3\}$	$(\binom{n}{2} - 9)N_1 + 9N_3$
$\{(3)^{10}\}$	$\{5, (3)^7\}$	$\{(5)^2, (3)^4\}$	$\{(5)^3, 3\}$	$\{7, (3)^4\}$	$(\binom{n}{2} - 10)N_1 + 10N_3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Distinct values of $K'(A)$ that lie next to each other horizontally are known to yield the same value for $M(A)$. Furthermore, even for a particular value of $K'(A)$ there may exist multiple possibilities for the inner product structure of A. For example, if A is known to have $K'(A) = \{3, 3\}$ (or $\{(3)^2\}$), then without loss of generality we may assume $a_1 \cdot a_2 = a_1 \cdot a_3 = 3$

or $a_1 \cdot a_2 = a_3 \cdot a_4 = 3$, each yielding distinct matrices under Theorem 2.3.4. No doubt, the total enumeration of the possible values of $K'(A)$ for a matrix A satisfying $M(A) > M(A_b)$ is a very challenging task. If one is to show that A_b successfully attains $M(A_b) = M_n^*$, then proof must be found that no matrix A exists such that $K'(A)$ represents a set listed higher than $K'(A_b)$ in the above table.

Luckily, for the $n = 9$ case, there are only a few cases to consider. As seen by the above table, we note that a matrix in row 4 has already been found, namely, A_9 has $K'(A_9) = \{5\}$. Therefore, we must show that no matrix B with $K'(B) = \{3\}$ or $K'(B) = \{3, 3\}$ exists. To accomplish this task, the program `CreateCE.m` is designed to attempt to construct such a matrix B by sequential additions to a given initial matrix. See the section on Computer Programs for details about the construction technique. The sets of input parameters:

$$A = \begin{pmatrix} + & + & + & + & + & + & + & + & + \\ + & + & + & + & + & - & - & - & - \\ + & + & + & - & - & + & + & - & - \end{pmatrix}$$

with

$$(1)\ v = (\,120, 200, 300, 420, 560, 718\,)$$

$$(2)\ v = (\,120, 200, 300, 420, 560, 716\,)$$

$$(3)\ v = (\,120, 200, 300, 420, 558, 716\,)$$

correspond to attempts to create matrices with $K'(A) = \{3\}, \{3, 3\}$, and $\{3, 3\}$, respectively. Each yields no final solutions, so $M(A_9) = M_9^*$. Furthermore, although the proof is not extended to include other values of $n = 4k + 1$, we mention that $\det(A_9) = D_n^*$, see [8].

13×13 case

According to Theorem 2.4.8, an *Ehlich*-type matrix may exist for $n = 13$. Although an example is given in [8], we shall illustrate again the construction technique previously described.

Under the conditions of Theorem 2.3.4, we again assume

$$a_1 = (\underbrace{+ \ \cdots \ +}_{13})$$

and that $a_1 \cdot a_i = 1$ for $2 \leq i \leq 13$. Furthermore, we assume

$$a_2 = (\underbrace{+ \ \cdots \ +}_{7} \ \underbrace{- \ \cdots \ -}_{6})$$

Consider row 3. Let k represent the number of 1's that are to be placed in columns 1 through 7. Therefore, under our assumption that $a_1 \cdot a_3 = 1$, we are left with the following diophantine equation:

$$\begin{aligned} \pm 1 &= a_2 \cdot a_j \\ &= k - (7-k) - (7-k) + (6 - (7-k)) \\ &= 4k - 15 \end{aligned}$$

Note that no integer value of k exists such that $a_2 \cdot a_3 = -1$. Consequently, up to permutation similarity we may assume rows a_1, a_2, and a_3 are of the form:

$$A = \begin{bmatrix} + & + & + & + & + & + & + & + & + & + & + & + & + \\ + & + & + & + & + & + & + & - & - & - & - & - & - \\ + & + & + & + & - & - & - & + & + & + & - & - & - \end{bmatrix}$$

To continue this construction process, consider the addition of a_4 such that $a_4 \cdot a_i = 1$ $\forall\ i \in \{1,2,3\}$. At this iteration, however, we split the columns of A into four disjoint sets of equal columns: $s_1 = \{1,2,3,4\}, s_2 = \{5,6,7\}, s_3 = \{8,9,10\}, s_4 = \{11,12,13\}$. Let k_i represent the number of 1's in row 4 with column indices in s_i, which implies the following set of constraints from logic previously explained:

$$\begin{aligned} k_1 + k_2 &= 4 \\ k_1 + k_3 &= 4 \\ k_1 + k_2 + k_3 + k_4 &= 7 \end{aligned}$$

Subtracting the second constraint from the first implies that $k_2 = k_3$. Therefore, we are left with the following four possibilities for a_4:

k_1	k_2	k_3	k_4	a_4
4	0	0	3	$[++++---------+++]$
3	1	1	2	$[+++-+--+--++-]$
2	2	2	1	$[++--++-++-+--]$
1	3	3	0	$[+---++++++---]$

The first case may be ruled out due to the fact that it adds the constraint $k_1 + k_4 = 4$, which yields no feasible solutions for adding a fifth row that has inner product 1 with all previous rows. Therefore, we are left with the remaining three cases. Using the parameters

$$A = \begin{pmatrix} a_1 & a_2 & a_3 & a_4 \end{pmatrix}^t$$

with a_4 from the case where $k_1 = 1$ and $k_2 = k_3 = 3$, and

$$v = (420, 630, 882, 1176, 1512, 1890, 2310, 2772, 3276)$$

the program `CreateCE.m` yields the matrix A_{13} given in Appendix A. A_{13} is *Ehlich*-type, "nearly-perfect", and attains $M(A_{13}) = M_{13}^*$ and $\det(A_{13}) = D_n^*$.

Unfortunately, the preliminary construction and complementary computational techniques described for the $n = 9$ and $n = 13$ case are limited. For $n = 17$, for example, the complete enumeration of possible row additions is not easily handled by a computer. A more sophisticated search algorithm is required to help raise the lower bounds for M_n^* with $n = 4k + 1$ and $k > 4$. We discuss this topic in the following section.

2.5 Improving Search Heuristics

Although we are not able to prove optimality for the matrices A that attain the best value currently known for $M(A)$ in this section, we provide two effective heuristic algorithms that can be used for Problem 1.

2.5.1 Discrete Improving Search

The problem of finding the true value of M_n^* can be characterized as a large combinatorial optimization problem with a nonlinear objective function. Furthermore, as we have seen, the problem is too large for total enumeration of possible solutions. Therefore, consider the following discrete improving search algorithm; see [13].

Algorithm 2.5.1: Discrete Improving Search

Step 0: Choose any $A^{(0)} \in \mathcal{A}_n$ as an initial solution and set index $t = 0$.

Step 1: If no move $\Delta_{i,j}A$ in the move set M is improving, then stop. $A^{(t)}$ is the best solution found.

Step 2: Choose some improving move in M as $\Delta_{i,j}A^{(t+1)}$.

Step 3: Update: $A^{(t+1)} \leftarrow A^{(t)} \cdot \Delta_{i,j}A^{(t+1)}$

Step 4: Increment $t \leftarrow t + 1$ and return to Step 1.

In general, the move set M for this problem is a set of elements corresponding to a distinct change in the entries of matrix $A^{(t)}$ that yields a feasible solution, i.e. a matrix $A^{(t+1)} \in \mathcal{A}_n$. In our search, we let M denote the set of moves corresponding to the multiplication of a single entry in $A^{(t)}$ by -1. We shall call one such move $(\Delta_{i,j}A^{(t+1)})$ to be the "flip" of a bit (the entry $a_{i,j}$) in $A^{(t)}$. Consequently, at any given interation there are n^2 moves in M. The operator $(\cdot)$ maps the sets $\mathcal{A}_n$ and M into $\mathcal{A}_n$. More specifically, the operation $A^{(t)} \cdot \Delta_{i,j}A^{(t+1)}$ yields the matrix $A^{(t+1)}$ which has all entries equal to $A^{(t)}$ except for the flipped $a_{i,j}$ entry.

Consider the following definition; see [13]:

Definition 2.5.1 *A solution x is a local optimum if all moves from x in the move set M produce either an infeasible solution or a solution with an objective function value that is inferior to that of x.*

Note that no move in our algorithm can produce a matrix $A^{(t+1)}$ that is infeasible, i.e. $A^{(t+1)}$ is guaranteed to be a member of $\mathcal{A}_n$. We see that all final solutions found by Algorithm 2.5.1 are local optimum. However, it is well known that for problems of this type local optima are not necessarily global optima, i.e. if $A^{(f)}$ denotes the final solution given by Algorithm 2.5.1, then $M(A^{(f)})$ is not necessarily equal to M_n^*.

Although Algorithm 2.5.1 is not very complex, it provides a good starting point for the development of a more advanced improving search heuristic. Ideally, our search will be able to tighten the bounds for M_n^* for $n = 4k + 1$ to a point where all possible better solutions are known to be infeasible. Infeasible solutions in this instance refer to those values of $M(A)$ such that no $A \in \mathcal{A}_n$ exists. We now have a relatively easy method to find if there are ways to increase the value of $M(A)$ by flipping a single entry in the matrix A.

As a final addition to the algorithm, a common technique is to start from multiple starting solutions as an attempt to broaden the search space over a wider range of matrices in $\mathcal{A}_n$, see [13]. The table below illustrates the best values of $M(A)$ found using this "Multistart Search" addition to Algorithm 2.5.1. Furthermore, we would like to compare the effectiveness of using the "Multistart Search" approach versus a single run of the algorithm. As a simple starting solution for this run, we consider the case when $A^{(0)} = 2I_n - J_n$ where I_n is the $n \times n$ identity matrix. For $n = 3, 4,$ and 5 this matrix is known to be optimal. However, for large n this matrix is known to be far from optimal, so the selection of it as a generic starting solution is arbitrary for the most part. Let S represent the final value of $M(A)$ when the algorithm is run with $A^{(0)} = 2I_n - J_n$ where I_n is the $n \times n$ identity matrix. The remainder of the search uses random matrices as initial starting solutions. In other words, for each individal replication of the algorithm, the starting solution is created as a matrix $A \in \mathcal{A}_n$ with an equal probability of having a -1 or a 1 in each position. Let "Avg. $M(A)$" denote the average value of $M(A)$ over 100 replications using random matrices. Finally, $M(A^*)$ represents the best value found over the entire search, U represents the theoretical upper bound when A is of *Ehlich*-type, and the '%' column stores the percentage that $M(A^*)$ rests below U.

Table 2.5.1

n	S	Avg. $M(A)$	$M(A^*)$	U	%
17	9708	9714.58	9760	9792	0.33%
21	22282	22937.70	22994	23100	0.46%
25	41248	46520.70	46600	46800	0.43%
41	180968	341297.2	341618	344400	0.81%

Here we note that the cases where $n = 25$ and $n = 41$ are of particular interest due to the fact that a *Ehlich*-type matrix may exist in each case. Although an example of each is unknown, the creation of such a matrix through improving search techniques would both (1) be easy to prove as the optimal matrix for the given size n, and (2) illustrate the effectiveness of a more advanced heuristic.

2.5.2 Tabu Search

In the discrete improving search Algorithm 2.5.1 given previously in this section, our search was limited due to the fact that final solutions are given as the first matrix $A^{(t)}$ for which there are no improving moves $\Delta_{i,j}A^{(t+1)}$. The "Tabu Search" heuristic is designed to escape local optima and allow the search to explore a wider range of the search space. At the core of Tabu Search is a short-term memory process, see [7], that allows the search algorithm to accept non-improving moves while attempting to avoid the risk of "cycling", i.e. returning right back to a previous local optima. Consider the following algorithm with notation similar to that of Algorithm 2.5.1; see [7], [13].

Algorithm 2.5.2: Tabu Search

Step 0: Choose any initial $A^{(0)}$ as an initial solution, set iteration limit t_{max}, index $t = 0$, $tabu\_list = \emptyset$, $list\_length = L$, and incumbent solution $A^* \leftarrow A^{(0)}$.

Step 1: If $t = t_{max}$, then stop. A^* is the best solution found.

Step 2: Choose some non-tabu move $\Delta_{i,j}A$ in the move set M as $\Delta_{i,j}A^{(t+1)}$.

Step 3: Update: $A^{(t+1)} \leftarrow A^{(t)} \cdot \Delta_{i,j}A^{(t+1)}$

Step 4: If the value $M(A^{(t+1)}) > M(A^*)$, then set $A^* \leftarrow A^{(t+1)}$.

Step 5: Remove any elements of *tabu_list* that have been a member of it for at least *list_length* iterations. Add $\Delta_{i,j}A^{(t+1)}$ to *tabu_list*.

Step 6: Increment $t \leftarrow t + 1$ and return to Step 1.

Again, we note that no move in the move set M will yield an infeasible solution. Therefore, termination of the algorithm relies strictly on the iteration limit t_{max}. The variables *tabu_list* and *list_length* are used to prevent the search from selecting a move that will allow examination of a previously considered local optimum. In other words, if *list_length* is sufficiently long, then enough moves will be set as "tabu" so that the algorithm will be unable to retrace its steps and consider a matrix $A^{(t+1)}$ that is equal to some previously considered $A^{(i)}$, $0 \leq i < t + 1$. Many additional features can be added to any given Tabu Search algorithm; see [7], [13]. For example, the concept of "aspiration criteria" is one designed to let the algorithm override the "tabu" status of a move if the acceptance of that move will yield a solution $A^{(t+1)}$ with $M(A^{(t+1)}) > M(A^*)$, i.e. it will produce a matrix that represents the best solution yet found. In our experiments, however, no better solutions were found by including an aspiration criterion.

Two distinct *tabu_list*s were used in our experiments: one that disallows the search to reflip an unique bit for $list\_length_1$ iterations and one that disallows two bits in the same row to be flipped within $list\_length_2$ iterations. Furthermore, in our implementation the move accepted during each iteration represents either the best improving move or else the least non-improving move over the entire set of moves in M that are currently non-tabu. We performed a variety of experiments on Problem 1 for the cases where $n = 17, 21, 25$, and 41. Similar to the "Multistart Approach" mentioned previously, one experiment was run for each case with an initial solution equal to the matrix $2I_n - J_n$. In additon, 100 replications were run with random matrices as initial solutions. As an initial test, each replication was run for $\frac{n^2}{2}$ rounded up to the nearest 100 iterations. The results of these experiments with a variety of values for the *list_lengths* of the two *tabu_list*'s are given in Appendix B. The best instances of each, i.e. those that yield the best solution found over all searches and attain the maximum average value for $M(A)$, are given in the table below.

Table 2.5.2

n	S	Avg. $M(A)$	$M(A^*)$	U	%
17	9768	9763.64	9768	9792	0.25%
21	23016	23026.6	23076	23100	0.10%
25	46648	46650.5	46674	46800	0.27%
41	343512	343567	343636	344400	0.22%

When compared to the data in Table 2.5.1, we note that the Tabu Search algorithm was able to find better solutions for both the best and the average case. Although we cannot conclude that a single run of Algorithm 2.5.2 will always yield a better solution than Algorithm 2.5.1, we can easily see the benefits of a more advanced heuristic when multiple runs are considered.

Finally, as an extension of the relative "best" sets of parameters for $list\_length_1$ and $list\_length_2$ for each case, a longer experiment of 1000 replications was run for each. Statistics for these experiments are given below.

Table 2.5.3

n	Avg. $M(A)$	$M(A^*)$	U	%
17	9764.62	9768	9792	0.25%
21	23025.0	23076	23100	0.10%
25	46652.8	46694	46800	0.23%
41	343574	343648	344400	0.22%

Unfortunately, no significant improvement is found when considering ten times as many replications. This could imply that either (1) many solutions found after 100 replications are optimal, or (2) an extension of the given Algorithm 2.5.2 is needed to better the search. We leave consideration of this to further research.

As a final note, it is unclear whether or not there is a strong connection between the solutions for Problem 1 and Problem 2 for large n. When compared to the matrices in [8], we find that the best solution found in the $n = 17$ case, call it A_{17}, has $\det(A_{17}) \neq D^*_{17}$ due to the fact that the matrix A attaining $\det(A) = D^*_{17}$ has fewer odd submatrices than A_{17}. On the other hand, the best solution found in the $n = 21$ case has the same determinant as that of the matrix A_{21} satisfying $\det(A_{21}) = D^*_{21}$. Of course, it remains to be seen whether or not either of these matrices is optimal for Problem 1 and any mention of the connection between the two problems in these cases would be speculative. We do note, however, that if an *Ehlich*-type matrix A exists, then $M(A) = M^*_n$ and $\det(A) = D^*_n$.

2.6 Computer Programs

All programs provided in this section are written in code for MatLab and/or C/C++.

1. num_even_submatrices.m

   A simple program to compute $M(A)$ for a given matrix A according to Equation 2.3.1.

2. multistart.cc

   A discrete improving search algorithm designed to perform a sequence of improving "moves" on a matrix A until a local optimum is reached.

3. pad_Hadamard_search.m

   A program that considers all possible row and column additions to a matrix $B \in \mathcal{A}_{n-1}$ in order to provide a lower bound for the value M^*_n.

4. tabu_search.cc

   A Tabu Search algorithm designed to improve the lower bound of M^*_n for specific values of n. Program was specifically used in this chapter to experiment on the values $n = 17, 21$, and 25.

5. CreateCE.m

   With some previous knowledge of the possible value of M^*_n for a given value of n, this program can be used to find a counterexample that the known value is optimal. In conjunction with Table 2.4.1, an exhaustive search can be used to create a matrix that would attain a larger number of odd submatrices than the current best solution found. The algorithm is described as follows.

   First, up to permutation similarity, attempt to define as many rows of the matrix A, say row a_1 through a_i, as possible (similar to methods previously used in the 9×9 and 13×13 subcases). In some cases, defining as many of the rows with inner product equal to ± 1 seems to be beneficial while in other cases it seems to be better to define the more "non-perfect" rows. Next, define the vector v with entry i equal to the desired number of odd submatrices in the matrix , $(a_1 \ \ldots \ a_i \ a_{i+1})$, i.e. after the addition of the $(i+1)$th row. The program begins with the input matrix A and attempts to add row after row with each addition satisfying the desired number of odd submatrices specified in v. Certain steps have been taken to minimize the run-time of the program, as it is an exhaustive search, but these methods will not be described. Essentially, the program creates a tree structure where matrices in the ith level satisfy the desired number of odd submatrices in the ith entry of v. If for a particular matrix there exists no possible row addition that will provide the desired value $v(i)$, then the search terminates consideration of this matrix. Therefore, a matrix exists with the final number of desired odd submatrices only if one or more branches does not terminate until after the addition of the nth row of the matrix.

2.7 Further Research

A variety of points still remain open for both Problems 1 and 2. For example, the true value of M_n^* is still unknown for many large values of $n = 4k+1$. Our computer experiments were able to yield final solutions that attain a total number of odd submatrices within a fraction of one percent of the theoretical optimum, but still the proof of their optimality remains open. Furthermore, if a straightforward proof does not exist for a general class of matrices in this case, then are there yet other techniques that yield a better bound on the value of M_n^*? Certainly, the augmentation of Hadamard matrices of order $n-1$ is known to provide a good starting point for this technique.

Table 2.7.1

n	$eig(A^tA)$
3	$\{1,4,4\}$
4	$\{4,4,4,4\}$
5	$\{4,4,4,4,9\}$
6	$\{2,2,8,8,8,8\}$
7	$\{1,8,8,8,8,8,8\}$
8	$\{8,8,8,8,8,8,8,8\}$
9	$\{4, \frac{29}{2} - \frac{\sqrt{57}}{2}, \frac{29}{2} + \frac{\sqrt{57}}{2}, 8,8,8,8,8,8\}$
10	$\{2,2,12,12,12,12,12,12,12,12\}$
11	$\{1,12,12,12,12,12,12,12,12,12,12\}$
12	$\{12,12,12,12,12,12,12,12,12,12,12,12\}$
13	$\{12,12,12,12,12,12,12,12,12,12,12,12,25\}$
14	$\{2,2,16,16,16,16,16,16,16,16,16,16,16,16\}$
15	$\{1,16,16,16,16,16,16,16,16,16,16,16,16,16,16\}$
16	$\{16,16,16,16,16,16,16,16,16,16,16,16,16,16,16,16\}$

As we have seen throughout our study, the structures of matrices A attaining $M(A) = M_n^*$ are very attractive. As a further illustration of this fact, consider Table 2.7.1. All entries in this table are drawn from matrices known to satisfy $M(A) = M_n^*$ and some, see Appendix A, are known to also attain $\det(A) = D_n^*$. Is there more to be said about the eigenvalue structure of matrices attaining optimal values for these problems? Certainly, the significance of Hadamard matrices seems to extend even to neighboring cases of the value of n. Will all cases for $n = 4k + 1$ where an *Ehlich*-type matrix does not exist yield non-integer values in $eig(A^tA)$?

As described in our discussion of improving search heuristics, these problems can be defined in terms of a large combinatorial optimization problem with a nonlinear objective function. Along these lines, another possible approach is to characterize these problems in terms of the maximization problem:

$$\begin{aligned} \max f(A) &= \operatorname{tr} C_k(A^tA) \\ s.t. \quad & a_{i,j} \in \{-1, 1\}, 1 \leq i \leq m, 1 \leq j \leq n \end{aligned}$$

In other words, the problem can be considered with integer programming techniques. To this effect, the relaxation of the constraints to consider matrices with entries in the closed set $[-1, 1]$ may open new doors in the study of these problems.

As a final note, experimentation with improving search heuristics suggests that further development of these techniques could provide better lower bounds for unknown cases. Furthermore, through the experiments mentioned during this report, we find that evidence to suggest that the Tabu Search heuristic is able to find a near-optimal solution in all of the mentioned cases, i.e. solutions to within a fraction of a percent of the theoretical optimum. The proof that such a condition holds for any n would suggest that a version of this improving search algorithm could always be used to create near-optimal solutions for large unknown cases.

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Appendix A

Matrices A_n satisfying $M(A_n) = M_n^*$

The following table lists the maximum number of odd submatrices for small values of n, found throughout our research. We list only square matrices $A \in \mathcal{A}_n(\{-1, 1\})$.

n	$\max_{A \in \mathcal{A}_n} M(A)$	$M(A) = M_n^*$?	Attains D_n^*?
2	1	$\surd$	$\surd$
3	6	$\surd$	$\surd$
4	24	$\surd$	$\surd$
5	60	$\surd$	$\surd$
6	129	$\surd$	*sometimes*
7	252	$\surd$	X
8	448	$\surd$	$\surd$
9	714	$\surd$	$\surd$
10	1105	$\surd$	*sometimes*
11	1650	$\surd$	X
12	2376	$\surd$	$\surd$
13	3276	$\surd$	$\surd$
17	9768	*unknown*	X
21	23076	*unknown*	*most likely*
25	46674	*unknown*	*unknown*
41	341618	*unknown*	*unknown*

Matrices A_n attaining $\max_{A \in \mathcal{A}_n} M(A)$:

$$A_2 = \begin{pmatrix} + & + \\ + & - \end{pmatrix} A_3 = \begin{pmatrix} + & + & + \\ + & + & - \\ + & - & + \end{pmatrix} A_4 = \begin{pmatrix} + & + & + & + \\ + & + & - & - \\ + & - & + & - \\ + & - & - & + \end{pmatrix}$$

$$A_5 = \begin{pmatrix} + & + & + & + & + \\ + & + & - & - & - \\ + & - & + & - & - \\ + & - & - & + & - \\ + & - & - & - & + \end{pmatrix} A_6 = \begin{pmatrix} + & - & + & - & - & - \\ - & + & - & + & - & - \\ - & - & - & - & + & + \\ + & - & - & + & - & + \\ - & + & + & - & - & + \\ - & - & + & + & + & - \end{pmatrix}$$

$$A_7 = \begin{pmatrix} + & + & + & + & + & + & + \\ + & + & + & - & + & - & - \\ + & + & - & + & - & + & - \\ + & + & - & - & - & - & + \\ + & - & + & + & - & - & + \\ + & - & + & - & - & + & - \\ + & - & - & - & + & + & + \end{pmatrix} A_8 = \begin{pmatrix} + & + & + & + & + & + & + & + \\ + & + & + & - & + & - & - & - \\ + & + & - & + & - & + & - & - \\ + & + & - & - & - & - & + & + \\ + & - & + & + & - & - & + & - \\ + & - & + & - & - & + & - & + \\ + & - & - & + & + & - & - & + \\ + & - & - & - & + & + & + & - \end{pmatrix}$$

$$A_9 = \begin{pmatrix} + & + & + & + & + & + & + & + & + \\ + & + & + & - & + & - & - & - & - \\ + & + & - & + & - & + & - & - & - \\ + & + & - & - & - & - & + & + & - \\ + & - & + & + & - & - & + & - & - \\ + & - & + & - & - & + & - & + & - \\ + & - & - & + & + & - & - & + & - \\ + & - & - & - & + & + & + & - & - \\ + & - & - & - & - & - & - & - & + \end{pmatrix}$$

$$A_{10} = \begin{pmatrix} + & - & + & - & - & - & + & + & + & - \\ + & + & - & + & - & - & - & + & + & + \\ - & + & + & - & + & - & - & - & + & + \\ + & - & + & + & - & + & - & - & - & + \\ + & + & - & + & + & - & + & - & - & - \\ + & + & + & - & + & + & - & + & - & - \\ - & + & + & + & - & + & + & - & + & - \\ - & - & + & + & + & - & + & + & - & + \\ - & - & - & + & + & + & - & + & + & - \\ + & - & - & - & + & + & + & - & + & + \end{pmatrix}$$

$$A_{11} = \begin{pmatrix}
+ & - & + & - & - & - & + & + & + & - & + \\
+ & + & - & + & - & - & - & + & + & + & - \\
- & + & + & - & + & - & - & - & + & + & + \\
+ & - & + & + & - & + & - & - & - & + & + \\
+ & + & - & + & + & - & + & - & - & - & + \\
+ & + & + & - & + & + & - & + & - & - & - \\
- & + & + & + & - & + & + & - & + & - & - \\
- & - & + & + & + & - & + & + & - & + & - \\
- & - & - & + & + & + & - & + & + & - & + \\
+ & - & - & - & + & + & + & - & + & + & - \\
- & + & - & - & - & + & + & + & - & + & +
\end{pmatrix}$$

$$A_{12} = \begin{pmatrix}
+ & - & - & - & - & - & - & - & - & - & - & - \\
+ & + & - & + & - & - & - & + & + & + & - & + \\
+ & + & + & - & + & - & - & - & + & + & + & - \\
+ & - & + & + & - & + & - & - & - & + & + & + \\
+ & + & - & + & + & - & + & - & - & - & + & + \\
+ & + & + & - & + & + & - & + & - & - & - & + \\
+ & + & + & + & - & + & + & - & + & - & - & - \\
+ & - & + & + & + & - & + & + & - & + & - & - \\
+ & - & - & + & + & + & - & + & + & - & + & - \\
+ & - & - & - & + & + & + & - & + & + & - & + \\
+ & + & - & - & - & + & + & + & - & + & + & - \\
+ & - & + & - & - & - & + & + & + & - & + & +
\end{pmatrix}$$

$$A_{13} = \begin{pmatrix}
+ & + & + & + & + & + & + & + & + & + & + & + & + \\
+ & + & + & + & + & + & + & - & - & - & - & - & - \\
+ & + & + & + & - & - & - & + & + & + & - & - & - \\
+ & - & - & - & + & + & + & + & + & + & - & - & - \\
- & + & + & - & + & + & - & + & + & - & + & - & - \\
- & + & + & - & + & - & + & + & - & + & - & + & - \\
- & + & + & - & - & + & + & - & + & + & - & - & + \\
- & + & - & + & + & + & - & + & - & + & - & - & + \\
- & - & + & + & + & + & - & - & + & + & - & + & - \\
- & + & - & + & - & + & + & + & + & - & - & + & - \\
- & - & + & + & - & + & + & + & - & + & + & - & - \\
- & - & + & + & + & - & + & + & + & - & - & - & + \\
- & + & - & + & + & - & + & - & + & + & + & - & -
\end{pmatrix}$$

Appendix B

Tabu Search Results

The following table of results for the 17×17 case of Problem 1 are based on 200 iterations and an initial seed of 123456789.

$list\_length_1$	$list\_length_2$	I	Avg. $M(A)$	$M(A^*)$
50	8	9742	9748.50	9768
50	5	9758	9753.18	9768
50	3	9750	9755.04	9768
50	1	9756	9756.92	9768
30	8	9746	9751.64	9768
30	5	9768	9757.70	9768
30	3	9760	9758.82	9768
30	1	9760	9761.78	9768
10	8	9760	9758.52	9768
10	5	9768	9761.78	9768
10	3	9760	9762.86	9768
10	1	9768	9763.64	9768
5	8	9760	9760.14	9768
5	5	9754	9760.04	9768
5	3	9760	9759.96	9768
5	1	9768	9761.46	9768

The following table of results for the 21×21 case of Problem 1 are based on 300 iterations and an initial seed of 123456789.

$list\_length_1$	$list\_length_2$	I	Avg. $M(A)$	$M(A^*)$
50	8	23002	23001.5	23020
50	5	23010	23006.8	23034
50	3	23010	23009.0	23054
50	1	23000	23007.3	23032
30	8	22992	23005.6	23024
30	5	22974	23010.5	23032
30	3	23000	23012.9	23050
30	1	23004	23012.5	23048
10	8	23014	23017.7	23076
10	5	23050	23019.4	23068
10	3	23018	23022.6	23076
10	1	23024	23023.1	23076
5	8	23000	23019.0	23076
5	5	23002	23022.0	23076
5	3	23016	23022.2	23076
5	1	23016	23026.6	23076

The following table of results for the 25×25 case of Problem 1 are based on 400 iterations and an initial seed of 123456789.

$list\_length_1$	$list\_length_2$	I	Avg. $M(A)$	$M(A^*)$
50	8	46610	46624.1	46652
50	5	46610	46626.7	46650
50	3	46632	46629.7	46656
50	1	46614	46628.8	46656
30	8	46612	46629.8	46650
30	5	46636	46633.4	46660
30	3	46620	46636.3	46664
30	1	46626	46638.2	46668
10	8	46630	46643.9	46668
10	5	46632	46649.5	46672
10	3	46640	46650.0	46668
10	1	46648	46650.5	46674
5	8	46634	46644.9	46664
5	5	46646	46645.1	46672
5	3	46640	46645.0	46674
5	1	46628	46644.1	46668

The following table of results for the 41×41 case of Problem 1 are based on 900 iterations and an initial seed of 123456789.

$list\_length_1$	$list\_length_2$	I	Avg. $M(A)$	$M(A^*)$
50	8	343470	343506	343574
50	5	343480	343512	343570
50	3	343380	343527	343568
50	1	343378	343520	343566
30	8	343460	343532	343580
30	5	343446	343543	343592
30	3	343498	343546	343598
30	1	343394	343546	343608
10	8	343466	343560	343616
10	5	343512	343567	343636
10	3	343472	343572	343622
10	1	343388	343574	343624
5	8	343478	343562	343620
5	5	343510	343496	343604
5	3	343488	343520	343624
5	1	343410	343531	343616