# DETERMINANT OPTIMIZATION ON BINARY MATRICES

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SYNOPTIC ABSTRACT

Structural connections between $m \times n$ $(-1,1)$-matrices $A$ such that $A$ has the maximum number of $(2 \times 2)$-submatrices with nonzero determinant and $m \times n$ $(-1,1)$-matrices $B$ that maximize $\det(B^t B)$ are explored. The two types of matrices can be defined as solutions to two instances of the same optimization problem. The focus is on matrices satisfying the former property, specifically the most difficult case when $A$ is $n \times n$ with $n = 4k+1$, $k$ a natural number. Constructive approaches and a tabu search are developed and are found to provide near-optimal solutions for $13 < n \leq 41$. The best known solutions to date are found for $n = 4k+1 \leq 41$.

Key Words and Phrases: determinant, binary matrix, optimization, tabu search

## 1. INTRODUCTION

The primary focus of our work is to understand the structure of $(0,1)$-matrices with a maximum number of odd $(2\times 2)$-submatrices. An odd submatrix is one having the sum of its entries equal to an odd integer. As in many other optimization problems in combinatorial matrix theory, it is useful to convert a problem on $(0,1)$-matrices to a problem on $(-1,1)$-matrices simply by changing all zero entries to $-1$. In this case the conversion leads to an objective function in a more appealing analytic form. We can rephrase our problem as one involving determinants:

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

A $2\times 2$ $(-1,1)$-matrix has an odd number of ones if and only if it has a nonzero determinant. A second problem with determinants is:

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

Problems 1 and 2 are closely related to the study of Hadamard matrices. A Hadamard matrix has the maximum possible determinant (in absolute value) of any $n\times n$ complex matrix $A$ with elements $|a_{ij}|\leq 1$ (see Hadamard (1893) or Brenner and Cummings (1972)). Problems 1 and 2 are also related to certain optimal design problems in statistics (see Hedayat and Zhu (2003) and Hedayat et al. (1999)). For example, solutions to Problem 2 are D-optimal designs in the statistics literature. Other authors, such as those in Marks et al. (2003), have noted that Problem 1 is related to computing bounds on Turan numbers (see also deCaen et al. (1988)). While Problem 1 is thoroughly covered in Marks et al. (2003), we present different approaches to the problem including computational techniques that advance the study of the remaining unsolved case, namely, $n\times n$ matrices with $n=4k+1$, $k$ a natural number.

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 both Problems 1 and 2. Section 5 is devoted to computational techniques we developed. Finally, in Section 6 we present suggestions for further research on these problems.

The following notation will be used throughout the paper. Unless otherwise noted, all matrix entries are restricted to $-1$ and 1.

| | |
|---|---|
| $\mathcal{A}_{m,n},\mathcal{A}_n$: | the set of $m\times n$ and $n\times n$ matrices, respectively. |
| $M^*_{m,n},M^*_n$: | the maximum number of odd $(2\times 2)$-submatrices taken over the set $\mathcal{A}_{m,n}$ and $\mathcal{A}_n$, respectively. |
| $D^*_{m,n},D^*_n$: | the maximum determinant of matrices taken over the set $\mathcal{A}_{m,n}$ and $\mathcal{A}_n$, respectively. |
| $M(A)$: | the number of odd $(2\times 2)$-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 |
| $H_n$: | the set of Hadamard matrices of order $n$. |

## 2. COMPOUND MATRICES

Given an $m\times n$ matrix $A$ and $k\le\min\{m,n\}$, the $k$th 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. That is, submatrices corresponding to common row indices are ordered lexicographically based on column indices across a row of $C_k(A)$ and similarly for submatrices corresponding to common column indices. For example, if $A$ is $3\times 4$ and $d[i,j;k,l]$ denotes the determinant of the submatrix of $A$ lying in rows $i,j$ and columns $k,l$, then

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

Problem 1 reduces to the search for a matrix $A\in\mathcal{A}_{m,n}$ with the maximum number of nonzero entries in $C_2(A)$. Consider the following theorem.

**Theorem 1:** Let $A\in\mathcal{A}_{m,n}(\{-1,1\})$. Then,

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

**Proof.** Every odd $(2\times 2)$-submatrix in $A$ gives rise to an entry of $C_2(A)$ equal to $\pm 2$. Therefore, the total number of nonzero entries in $C_2(A) = [\mathrm{tr}C_2(A)C_2(A)^t]/4$. By properties of compound matrices,

$$\mathrm{tr}C_2(A)C_2(A)^t = \mathrm{tr}C_2(AA^t) = E_2(\lambda_1,\ldots,\lambda_m),$$

where $\lambda_1,\ldots,\lambda_m$ are the eigenvalues of $AA^t$, and

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

is the 2-elementary symmetric function (see Marshall and Olkin (1979) (section 19.F)). $\square$

By Theorem 1, Problems 1 and 2 can be formulated in terms of optimizing two instances of the same objective function. That is, Problems 1 and 2 can be rephrased as finding the maximum value of $\mathrm{tr}C_2(AA^t)$ and $\mathrm{tr}C_n(AA^t)$, respectively. In general, we have the following result.

**Theorem 2:** Suppose $S$ is the set of real $m\times n$ matrices $A$, $1 < m \le n$, such that $AA^t$ has diagonal entries all equal to $n$. For all $A \in S$,

$$\mathrm{tr}C_k(AA^t) \le E_k(m,\ldots,m)$$

with equality if and only if $AA^t = nI_m$.

**Proof.** Let $AA^t$ have eigenvalues $x_1 \ge x_2 \ge \cdots \ge x_m \ge 0$. Then $x_1 + x_2 + \cdots + x_m = tr(AA^t) = mn$, and

$$tr(AA^t) \equiv \sum_{1\le i_1<\cdots<i_k\le m} x_{i_1}\cdots x_{i_k},$$

see Marks et al. (2003) (section 19.F). By the theory of majorization (see Marks et al. (2003) section 4.A) the conclusion follows. $\square$

Thus, any $m\times n$ submatrix of an $n\times n$ Hadamard matrix is a solution to Problems 1 and 2. For further information on Hadamard matrices see `http://mathworld.wolfram.com/HadamardMatrix.html`.

## 3. COMBINATORIAL TECHNIQUES

Since a matrix $B$ satisfying $M(B) = M^*_{m,n}$ can be derived from a square matrix $A$ with $M(A) = M^*_n$ (see Marks et al. (2003)), we limit our attention to square matrices. The following theorem is proved in Marks et al. (2003).

**Theorem 3:** 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 1 or both $-1$. 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 $(2\times 2)$-submatrices over rows (columns) $i$ and $j$ is $k^+_{i,j} * k^-_{i,j}$.

By Theorem 3, the number of odd $(2\times 2)$-submatrices in $A$ is:

$$M(A) \quad = \quad \sum_{1\le i<j\le n} k^+_{i,j} * k^-_{i,j}. \tag{3.1}$$

There are many matrices with the same number of odd $(2\times 2)$-submatrices. The following theorem is proved in Marks et al. (2003).

**Theorem 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. Take the transpose.

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

3. Multiply any row or column by $-1$.

Upper and lower bounds on $M^*_n$ are easily established. First, $M(A) \ge 0$ for any $A \in \mathcal{A}_n$ with equality if and only if $A$ is equivalent to $J_n$ through the operations given in Theorem 4. For even $n$, the maximum number of odd $(2\times 2)$-submatrices within any pair $(i,j)$ of rows or columns is attained if and only if $k^+_{i,j} = k^-_{i,j} = n/2$. In this case, we say $(i,j)$ is a perfect pair (see Marks et al. (2003)). For odd $n$, the maximum number of odd $(2\times 2)$-submatrices within any pair $(i,j)$ of rows or columns is attained if and only if $k^+_{i,j} = (n+1)/2$ and $k^-_{i,j} = (n-1)/2$, or vice versa. In this case, we say $(i,j)$ is a near-perfect pair (see Marks et al. (2003)). In summary, bounds for $A \in \mathcal{A}_n$ are:

$$\text{n is even} \quad \Rightarrow \quad 0 \le M(A) \le \left(\frac{n}{2}\right)^2 \binom{n}{2}, \tag{3.2}$$

$$\text{n is odd} \quad \Rightarrow \quad 0 \le M(A) \le \left(\frac{n-1}{2}\right)\left(\frac{n+1}{2}\right)\binom{n}{2}. \tag{3.3}$$

If $a_i$ and $a_j$ are the $i$th and $j$th rows of $A$, respectively, then $k^+_{i,j} - k^-_{i,j} = a_i \cdot a_j$. Consequently, we have the following definition.

**Definition 1:** If the inner product of all pairs of rows in the matrix $A$ is equal to 0, then $A$ is perfect. If the inner product of all pairs of rows in the matrix $B$ is equal to $\pm 1$, then $B$ is near-perfect.

## 4. OPTIMAL SOLUTIONS

In this section, optimal solutions of Problem 1 are provided if we assume that the Hadamard Conjecture is valid. The problem can be split naturally into four distinct cases based on the value of $n$. For the first three cases, proofs of optimum values exist and are described along with some alternative approaches that have been considered. The final case, however, remains open for $n > 13$. In addition, throughout the proofs we make use of the fact that $\mathrm{eig}\left(BB^t\right)$ are the same as $\mathrm{eig}\left(B^tB\right)$.

### 4.1. $n = 4k$ and Hadamard Matrices

According to Theorem 2 and Definition 1, $A \in H_n$ attains $M(A) = M^*_n$, $\det(A) = D^*_n$, and $A$ is perfect. A large sample of Hadamard matrices can be found in Sloane. The structure of Hadamard matrices suggests that they can potentially be used to find matrices $A$ satisfying $M(A) = M^*_n$ for values of $n \neq 4k$ by adding or deleting the appropriate number of rows and columns. We consider this technique for the remaining cases.

## 4.2. $n = 4k - 1$

The optimum value $M_n^*$ for each $n$ in this case has been established in Marks et al. (2003). An alternative proof based on compound matrices is given below.

**Theorem 5:** Given $A \in H_{n+1}$, the matrix formed by the removal of any row and any column from $A$ is a matrix $B$ having a total of

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

odd $(2 \times 2)$-submatrices. Furthermore, $B$ is near-perfect and $M(B) = M_n^*$.

*Proof.* Let $A \in H_{n+1}$, so

$$\mathrm{eig}\,(A^t A) = \{\underbrace{n+1, \ldots, n+1}_{n+1}\}.$$

Perform the necessary operations from Theorem 4 so that each entry of row $i$ and column $j$ is 1. The matrix $B$ obtained via the removal of row $i$ and column $j$ satisfies:

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

The eigenvalues of the first and second term of the right-hand-side constitute the sets

$$S_1 = \{n+1, \ldots, n+1\} \text{ and } S_2 = \{n, \underbrace{0, \ldots, 0}_{n-1}\},$$

respectively. Consequently,

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

and

$$\begin{aligned} M(B) &= \frac{1}{4} E_2(\mathrm{eig}\,(B^t B)) \\ &= \frac{1}{4}\left((n-1)(n+1) + \binom{n-1}{2}(n+1)^2\right) \\ &= \binom{\frac{n-1}{2}}{}\binom{\frac{n+1}{2}}{}\binom{n}{2}. \end{aligned}$$

$\square$

The only known cases for the value of $D_n^*$ where $n = 4k-1$ are $n = 3, 7$, and 11 (see Hedayat and Zhu (2003)). Of these only the matrix attaining $\det(A) = D_3^*$ satisfies $M(A) = M_3^*$. As far as we know there are no apparent connections between the matrices attaining optimal values for Problems 1 and 2 when $n = 4k-1$.

### 4.3. $n = 4k-2$

The optimum value $M_n^*$ for each $n$ in this case has been established in Marks et al. (2003). We sketch a proof of the following theorem using compound matrices.

**Theorem 6:** Given $A \in H_{n+2}$, a matrix $B$ formed by the removal of two rows and two columns from $A$ 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 $(2\times 2)$-submatrices.

*Proof.* Let $A \in H_{n+2}$. Without loss of generality, assume

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

where $a_i$ and $a_j$ are the $i$th and $j$th columns of $A$, respectively, and $+$ denotes 1 while $-$ denotes $-1$. The removal of $a_i$, $a_j$, one of the first $(n+2)/2$ rows, and one of the last $(n+2)/2$ rows of $A$ yields a matrix $B$ satisfying

$$B^tB = (n+2)I_n - J_n - \begin{pmatrix} J_{\frac{n+2}{2}-1} & -J_{\frac{n+2}{2}-1} \\ -J_{\frac{n+2}{2}-1} & J_{\frac{n+2}{2}-1} \end{pmatrix},$$

so

$$\begin{aligned} M(B) &= \frac{1}{4}E_2(\operatorname{eig}(B^tB)) \\ &= \frac{1}{4}E_2(\{2, 2, \underbrace{n+2, \ldots, n+2}_{n-2}\}) \\ &= \frac{1}{8}n^4 - \frac{1}{8}n^3 - \frac{1}{4}n^2 + \frac{n}{2}. \end{aligned}$$

$\square$

The approach described in Theorem 6 yields a matrix with the maximum number of odd $(2\times 2)$-submatrices, as seen by the following result (see Marks et al. (2003)).

**Theorem 7:** Let $A \in \mathcal{A}_n$ where $n = 4k-2$. The maximum number of odd $(2\times 2)$-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.

An interesting connection between solutions of Problems 1 and 2 is highlighted in the following theorem found in Heyadat and Zhu (2003).

**Theorem 8:** Let $n = 4k-2$, $k$ a natural number. An Ehlich-Wojtas-type matrix is a matrix $A \in \mathcal{A}_n$ satisfying

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

where $B = (n-2)I_m + 2J_m$, $m = n/2$. Such a matrix exists only if $2(n-1)$ is the sum of two perfect squares. Ehlich-Wojtas-type matrices satisfy $\det(A) = D_n^*$.

As a result of Theorem 7, Ehlich-Wojtas-type matrices are solutions to Problem 1. However, not all matrices formed by the method in Theorem 6 are Ehlich-Wojtas-type. Thus, the set of solutions to Problem 2 is a proper subset of that of Problem 1 in this case.

## 4.4. $n = 4k+1$

This is the most difficult case of Problem 1. Values of $M_n^*$ are known only for the small values of $n = 5$, 9, and 13. For each known value of $n$ we present constructive proofs of optimality. The construction technique augments a Hadamard matrix but becomes computationally burdensome for $n \geq 17$.

The preliminary bounds in Theorem 9 are given in Marks et al. (2003).

**Theorem 9:** If $A \in H_n$, 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:

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

The matrix $B$ in Theorem 9 is constructed by the addition of a row and column to $A$; details can be found in Marks et al. (2003). The difference in the bounds above is significant for large $n$, but the lower bound is tighter than the one obtained in Theorem 10 via the removal of three rows and columns from a Hadamard matrix.

**Theorem 10:** Given $A \in H_{4k+1}$ and $k \geq 1$, a matrix $B$ formed by the removal of three rows and three columns from $A$ attains a maximum of

$$M(B) = 32k^4 + 24k^3 + 2k$$

odd $(2 \times 2)$-submatrices.

*Proof.* Similar to the proofs of Theorems 5 and 6, the maximum number of odd $(2 \times 2)$-submatrices obtained by the removal of three rows and columns from $A \in H_{n+3}$ will be attained by a matrix $B$ satisfying

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

Moreover, $\operatorname{eig}(B^t B) = \{1, 4, 4, \underbrace{n+3, \ldots, n+3}_{n-3}\}$ and $M(B) = 32k^4 + 24k^3 + 2k$. $\square$

Thus, for $n = 4k+1$ the augmentation of a smaller Hadamard matrix provides better bounds than the decomposition of larger ones. However, this method may not always yield a solution to Problem 1. For example, the near-perfect matrix $A_{13}$ in Appendix A contains no $12 \times 12$ Hadamard submatrix. In the remainder of this section and in Section 5 we examine the structure of known solutions to $n = 4k+1$ and propose construction techniques unrelated to Hadamard matrices.

**5 by 5 case**

The matrix $A_5$ in Appendix A is near-perfect. The following theorem from Heyadat and Zhu (2003) describes the inner product structure of $A_5$ and the existence of other near-perfect matrices for this case.

**Theorem 11:** Let $A \in \mathcal{A}_n$, $n = 4k+1$, satisfying

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

be called an Ehlich-type matrix. Such a matrix exists only if $2n-1 = 8k+1$ is the square of an integer.

A near-perfect matrix $A$ of order $n = 4k+1$ exists if and only if $A$ is Ehlich-type. In Heyadat and Zhu (2003), Ehlich-type matrices are shown to also be solutions to Problem 2.

**9 by 9 case**

By Theorem 11, an Ehlich-type matrix does not exist for $n = 9$. However, the matrix $A_9$ in Appendix A is known to be a solution to Problem 1. The construction technique for $A_9$ is described with the hope that it may prove useful for larger values of $n = 4k+1$.

Assume $M_9^*$ is unknown. Theorem 9 yields $714 \le M_9^* \le 720$ and a matrix $A_9$ with $M(A_9) = 714$ is known; see Appendix A. If $A \in \mathcal{A}_9$ exists with $M(A) > M(A_9)$, then one of the following two properties holds. Either

(P1) $A$ is near-perfect, or

(P2) $A$ has exactly $k \in \{1, 2\}$ pairs of rows with inner product $\pm 3$ while the remaining pairs have inner product $\pm 1$.

Such a matrix would have $M(A)$ equal to 716, 718, or 720, respectively. A Ehlich-type matrix does not exist, so $M(A_9) = M_9^*$ if and only if matrices with property (P2) do not exist.

If a matrix $A$ with property (P2) exists, then it must have a set $P$ of at least $n-2 = 7$ rows such that $(i, j)$ is near-perfect for all distinct $s, t \in P$. Let $A = [a_1\ a_2\ \ldots\ a_9]^t$, then by Theorem 4 assume

$$a_1 = \begin{pmatrix} + & + & + & + & + & + & + & + & + \end{pmatrix}$$

and that $a_1 \cdot a_i = 1$ for all $2 \leq i \leq 9$, or else multiply row $a_i$ by $-1$. Furthermore, assume

$$a_2 = \begin{pmatrix} + & + & + & + & + & - & - & - & - \end{pmatrix}$$

so $a_2 \cdot a_j = \pm 1$ for all $3 \leq i \leq 9$. For $a_j$ with $3 \leq j \leq 9$, $a_1 \cdot a_j = 1$ so $a_j$ consists of four $-1$s and five 1s. If $k$ denotes the number of 1s in first five positions of $a_j$, then 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 $k$ is an integer, $k = 3$ and $a_2 \cdot a_j = 1$ for all $j \geq 3$. Up to permutation similarity, $A$ must have

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

The enumeration of all possible row additions to $(a_1\ a_2\ a_3)^t$ above may lead a matrix $A$ with $M(A) > M(A_9)$. Due to the specific inner product structure that such a matrix must possess, this enumeration is easily handled by a computer. Therefore, a viable construction technique is to set a goal value of $M(A)$, predetermine as many rows of $A$ as possible up to permutation similarity, and enumerate all possible additions for the remaining rows.

For $n = 9$, this procedure is not a hard one. In general, however, if $A^*$ yields the best known value for $M(A^*)$ for some $n$, then Table 1 illustrates the variety of possible sets of inner products that must be considered for the rows of a matrix $A$ with $M(A) > M(A^*)$. Let $K(A)$ denote the set of inner products of all pairs of rows $i$ and $j$, $i < j$, in $A$. 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 define

$$N_1 \equiv \left(\frac{n+1}{2}\right)\left(\frac{n-1}{2}\right), \;\; N_3 \equiv \left(\frac{n+3}{2}\right)\left(\frac{n-3}{2}\right).$$

Table 1. Possible sets of inner products

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

Distinct values of $K'(A)$ aligned horizontally in Table 1 yield the same value for $M(A)$. For a particular value of $K'(A)$ there may exist multiple possibilities for the inner product structure of $A$. For example, if $A$ has $K'(A)=\{(3)^2\}$, 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 4.

Following the guidelines of Table 1, a $9\times 9$ matrix with property (P2) must have $K'(B)=\{3\}$ or $K'(B)=\{(3)^2\}$. The program CreateCE.m performs the necessary enumeration of all possible row additions; see Section 5.3. The sets of input:

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

with

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

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

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

attempts to create matrices with $K'(A)=\{3\},\{(3)^2\}$, and $\{(3)^2\}$, respectively. Each attempt yields no final solutions, so $M(A_9)=M_9^*$.

Although the proof is not extended to include other values of $n=4k+1$, we mention $\det(A_9)=D_n^*$ (see Heyadat and Zhu (2003)).

**13 by 13 case**

An Ehlich-type matrix exists for $n = 13$ (see Heyadat and Zhu (2003)) for an example. The matrix $A_{13}$ in Appendix A is also Ehlich-type and was created via the construction technique described in 9 by 9 case in Section 4.4. Up to permutation similarity, we assume

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

and $a_4$ is one of

$$\begin{aligned} a_{4a} &= (+ + + + - - - - - - + + +), \\ a_{4b} &= (+ + + - + - - + - - + + -), \\ a_{4c} &= (+ + - - + + - + + - + - -), \\ a_{4d} &= (+ - - - + + + + + + - - -). \end{aligned}$$

With input $A = (a_1\ a_2\ a_3\ a_{4d})^t$ and

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

CreateCE.m produces $A_{13}$.

For $n \geq 17$, the complete enumeration of possible row additions is not easily handled by a computer because of the number of cases to consider. A more sophisticated search algorithm is required to raise the lower bounds for $M_n^*$ with $n = 4k+1$ and $k > 4$. Two such search algorithms are presented in following section.

## 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 heuristic algorithms that have proved effective for finding optimal or near-optimal solutions to Problem 1.

## 5.1. Discrete Improving Search

Problem 1 can be characterized as a large combinatorial optimization problem with a nonlinear objective function. The problem is too large for total enumeration of all possible solutions when $n \geq 17$, but discrete local improving search algorithms provide an alternative. These algorithms attempt to improve a given solution by making small changes (called moves) to the structure of the solution. A natural set of moves, $\Delta$, for Problem 1 is the multiplication of a single entry in $A^{(t)}$ by $-1$. A single move $\delta^t_{i,j} \in \Delta$ is a sign *flip* of entry $a_{i,j}$ of $A^{(t)}$, the current solution at iteration $t$. Such a move is improving if $M(A^(t+1)) = M(\delta^t_{i,j}(A^(t))) > M(A^(t))$. Consider the following definition.

**Definition 2:** A solution $x$ is a local optimum, with respect to $\Delta$, if all $\delta_{i,j} \in \Delta$ lead to either an infeasible solution or a solution with an objective function value inferior to that of $x$.

No move in $\Delta$ leads to a matrix $A^{(t+1)}$ that is infeasible. Therefore, if $A^{(f)}$ denotes the final solution found by Algorithm 1 below, then it must be a local optimum. There is no guarantee, however, that $M(A^{(f)}) = M_n^*$.

Algorithm 1: Discrete Improving Search

**Step 0:** Choose $A^{(0)} \in \mathcal{A}_n$. Set $t \leftarrow 0$.

**Step 1:** If no $\delta^t_{i,j} \in \Delta$ is improving, then stop. $A^{(t)}$ is the best solution found.

**Step 2:** Choose a most improving move in $\Delta$, $\delta^*_{i,j}$.

**Step 3:** Apply $\delta^*_{i,j}$ to $A^{(t)}$ yielding $A^{(t+1)}$. Return to Step 1.

A common technique to improve the quality of solutions found by Algorithm 1 is to begin from multiple starting solutions in an attempt to uncover multiple local optima. Table 2 records the best values of $M(A)$ found using this multistart implementation of Algorithm 1. $S$ denotes the value of $M(A^{(f)})$ when $A^{(0)} = 2I_n - J_n$. $2I_n - J_n$ is a reasonable starting solution for Algorithm 1 since $A_n = 2I_n - J_n$ is a global optimum for $n = 3, 4, 5$. The remainder of the starting solutions for Algorithm 1 are random matrices in which each entry is equally likely to be a 1 or $-1$. Avg. $M(A)$ denotes the average value of $M(A^{(f)})$ over 100 restarts with random matrices. $M(A^*)$ is the best value found. The column $U$ is the theoretical upper bound, assuming an Ehlich-type matrix exists, and '%' denotes the percentage that $M(A^*)$ lies below $U$.

Table 2. Best values of $M(A)$ with multistart

| 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% |

The cases where $n = 25$ and $n = 41$ are of particular interest since an $Ehlich$-type matrix may exist in each case, but an example for either case is unknown.

## 5.2. Tabu Search

In Algorithm 1 our search is terminated when we reach a matrix for which there are no improving moves in $\Delta$. Tabu search heuristics are designed to escape local optima, allowing a wider exploration of the search space, and have been shown to be highly competitive for a variety of discrete optimization problems (see Glover (1990) and Glover and Laguna (1998)). One key feature of a tabu search is a short-term memory list that allows the algorithm to accept non-improving moves while attempting to avoid cycling back to a previously explored local optimum. Consider the following algorithm with notation similar to that of Algorithm 1 (see Glover (1990)). $T$ denotes the tabu list and $L$ is its length.

Additional features can be added to any given tabu search algorithm (see Glover and Laguna (1998)). For example, an aspiration criteria allows the tabu status of a move to be overridden if the acceptance of that move yields the best solution yet found. In our experiments, however, no better solutions were found by including an aspiration criterion.

Algorithm 2: Tabu Search

**Step 0:** Select $A^{(0)} \in \mathcal{A}_n$ and $t_{max}$. Set $t \leftarrow 0$, $T \leftarrow \emptyset$, and $A^* \leftarrow A^{(0)}$.

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

**Step 2:** Find most improving (least non-improving) non-tabu move $\delta^t_{i,j} \in \Delta$. Label it $\delta^*_{i,j}$.

**Step 3:** Update $A^{(t+1)}$ by applying $\delta^*_{i,j}$ to $A^{(t)}$.

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

**Step 5:** Remove entries of $T$ whose tenure is at least $L$ iterations.

**Step 6:** Set $T \leftarrow T \cup \delta^*_{i,j}$, $t \leftarrow t+1$, and return to Step 1.

Two distinct tabu lists were used in our search. The first disallows moves that reflip the sign of an entry for $L_1$ iterations. The second disallows two signs in the same row to be flipped within $L_2$ iterations of each other. Appendix B provides a detailed summary of our experiments with multiple values of the tabu list lengths. Table 3 summarizes the results obtained with the best set of parameter values. As before, one instance of tabu search was initialized with $A^{(0)} = 2I_n - J_n$. An additional 100 restarts were initialized with random matrices. The columns of Table 3 record the same information as the columns in Table 2.

Table 3. Results with best set of parameter values

| 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% |

Our tabu search heuristic found better solutions (best and average) than our discrete improving search algorithm for all $n$ tested. Of course a single instance of Algorithm 1 may yield a better solution than a single instance of Algorithm 2.

However, the benefits of a tabu search are obvious when multiple restarts are considered. In addition, the second tabu list, which was inconsequential for $n = 17, 21, 25$ was critical in determining high quality solutions for $n = 41$ ($L_2 = 5$).

Finally, longer experiments with 1000 restarts were tested. The best set of tabu search parameters from the experiments in Table 3 were used in all 1000 restarts of the tabu search reported in Table 4. The column headings denote the same information as in Tables 2 and 3.

Table 4. Results from 1000 restarts of tabu search

| 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% |

Only small improvements were found (in boldface) for the 1000 restarts. This may imply that the solutions for $n = 17$ and 21 in Table 3 are optimal or that another approach is needed to uncover better solutions.

It remains unclear whether there is a strong connection between optimal solutions to Problem 1 and Problem 2 for large $n = 4k+1$. For example, the optimal solution to Problem 2 given in Heyadat and Zhu (2003) for $n = 17$ has fewer odd $(2 \times 2)$-submatrices than the best solution found with Algorithm 2. Consequently, the set of matrices that are optimal for Problem 1 and Problem 2 are disjoint in this case. However, the best solution for $n = 21$ found by Algorithm 2 has the same determinant as the optimal solution for Problem 2 given in Heyadat and Zhu (2003). If this solution is also optimal to Problem 1, then the solution sets overlap.

### 5.3. Computer Programs

All programs provided in this section are written in MatLab or C/C++. Many of these programs are available for download at `http://www.math.edu/~rrkinc/det.html`.

1. num_even_submatrices.m

   A simple program to compute $M(A)$ for a given matrix $A$ according to (3.1).

2. multistart.cc

   A discrete improving search heuristic: Algorithm 1.

3. tabu_search.cc

   A tabu search heuristic: Algorithm 2.

4. CreateCE.m

   Attempts to create a matrix $A'$ by appending rows to the input matrix $A$. Row additions are accepted if and only if the resulting matrix has $v(i)$ odd $(2 \times 2)$-submatrices after the addition of the $i$th row.

## 6. FUTURE RESEARCH

We have observed structural connections between the set of $m \times n$ $(-1, 1)$-matrices with the maximum number of $(2 \times 2)$-submatrices with nonzero determinant and those with the maximum value of $\det(A^t A)$. The sets of optimal solutions for both problems overlap for many values of $n$ and are tied closely to Hadamard matrices. In particular, the theory behind the existence of Ehlich-type and Ehlich-Wojtas-type matrices has proved useful for characterizing solutions for both problems. For the unsolved cases of Problem 1, solutions that attain objective values within a fraction of one percent of the theoretical optimal value using improving search heuristics were found. Thus, heuristic search techniques proved useful in uncovering near-optimal solutions when constructive techniques became computational burdensome (for $n \geq 17$).

In addition to their relationship with Hadamard matrices, optimal solutions to Problem 1 have other attractive structural properties. For example, consider the eigenvalues of $A_n A_n^t$ for the optimal matrices $A_n$, $n = 1, \ldots, 16$, found by the methods described in this paper; many of these matrices are given in Appendix A Table 5 gives these values in an appealing form. The repetitive eigenvalue structure of these solutions may provide further insight into the structure of optimal matrices to Problem 1.

Table 5. Eigenvalues of optimal matrices

| $n$ | $eig(A^tA)$ |
|---|---|
| 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 | $\{16,16,16,16,16,16,16,16,16,16,16,16,16,16,16,16\}$ |

Another approach for determining solutions to Problem 1 is to consider directly the discrete optimization problem:

$$\begin{aligned} \max f(A) &= \mathrm{tr} C_2(AA^t) \\ s.t. \quad & a_{i,j} \in \{-1,1\}, 1 \leq i \leq m, 1 \leq j \leq n \end{aligned}$$

In this form the problem can be attacked with traditional integer programming techniques. In addition, maximizing $f(A)$ over the linear relaxation of the constraints

$$-1 \leq a_{i,j} \leq 1,\ 1 \leq i \leq m,\ 1 \leq j \leq n$$

may provide high quality bounds and/or good starting solutions for the remaining unsolved cases.

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## APPENDIX A. MATRICES $A_n$ SATISFYING $M(A_n) = M_n^*$

Results for the set of $A_n$ in the solution set of Problem 1 found throughout our research.

| $n$ | $M(A_n)$ | $M(A_n) = M_n^*$? | $D(A_n) = D_n^*$? |
|---|---|---|---|
| 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 | 46694 | *unknown* | *unknown* |
| 41 | 343648 | *unknown* | *unknown* |

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

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

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

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

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

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

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

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

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

## APPENDIX B. TABU SEARCH RESULTS

$17 \times 17$: based on $t_{max} = 200$ and an initial seed of 123456789.

| $L_1$ | $L_2$ | $S$ | 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 |

$21 \times 21$: based on $t_{max} = 300$ and an initial seed of 123456789.

| $L_1$ | $L_2$ | $S$ | 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 |

$25 \times 25$: based on $t_{max} = 400$ and an initial seed of 123456789.

| $L_1$ | $L_2$ | $S$ | 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 |

$41 \times 41$: based on $t_{max} = 900$ and an initial seed of 123456789.

| $L_1$ | $L_2$ | $S$ | 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 |

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