LARGE-DETERMINANT SIGN MATRICES OF ORDER $4k + 1$.

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Abstract. The Hadamard maximal determinant problem asks for the largest $n \times n$ determinant with entries $\pm 1$. When $n \equiv 1 \pmod{4}$, the maximal excess construction of Farmakis & Kounias [FK] has been the most successful general method for constructing large (though seldom maximal) determinants. For certain small $n$, however, still larger determinants have been known; several new records were recently reported in [OSDS]. Here, we define “3-normalized” $n \times n$ Hadamard matrices, and construct large-determinant matrices of order $n + 1$ from them. Our constructions account for most of the previous “small $n$” records, and set new records when $n = 37, 49, 65, 73, 77, 85, 93$, and $97$, most of which are beyond the reach of the maximal excess technique. We conjecture that our $n = 37$ determinant, $72 \times 9^{17} \times 2^{36}$, achieves the global maximum.

1. Introduction

Overview. How big can the determinant of an $n \times n$ real matrix be, given a bound on the size of its entries? This is the Hadamard maximal determinant problem, and an easy argument reduces it to that of maximizing the determinant on matrices with entries $\pm 1$. From here on, we consider only such matrices$^1$. Determinant-maximizing matrices of this type are important in the design of experiments; they are called D-optimal designs.

When $n = 4k + 1$, the determinant of a $\pm 1$ matrix can never exceed the bound

\begin{equation}
B(n) := (n - 1)^{n - 1} \sqrt{2n - 1}
\end{equation}

due to Barba [Ba]. In these orders, the maximal excess construction of Farmakis & Kounias [FK] has offered the most successful general method for constructing determinants achieving a large fraction of $B(n)$. For certain orders such as $n = 13, 21, 25, 41$, and $61$, however, determinants beyond those attainable via maximal excess have been known for some time [Ra, CKM, Bh, BHH, Br]. In other dimensions, specifically $n = 29, 33, 45, 53, 69, 77, 85$ and $93$, a numerical ascent algorithm recently produced the largest known determinants [OSDS]. Here,

$^1$Maximizing the determinant of an $n \times n$ $\pm 1$ matrix is also equivalent to maximizing the determinant over $\{0, 1\}$-matrices of order $n - 1$. See [Wi].
we present a general construction which accounts for many of the cases above. A slight modification of our method accounts for the case $n = 29$. Except for certain maximizers which have been obtained as incidence matrices for suitable block designs ($n = 25, 41$ and $61$), this leaves only the current $n = 33$ record unexplained. In addition to clarifying the structure of many current records, our construction improves the previous records in dimensions $n = 77, 85$ and $93$, and sets new records in dimensions $n = 49, 65, 73$, and $97$. In a sequel to the present paper, we describe the modified construction which accounts for the case $n = 29$, and show that for $n = 37$, it produces the determinant $72 \times 9^{17} \times 2^{36} = 0.94B(37)$. We conjecture that this value achieves the global maximum in its dimension.

We base our construction on 3-normalized Hadamard matrices, which we define in §2 below. Starting with a 3-normalized Hadamard matrix of order $4k$, we make certain rank-1 modifications, and then construct a large-determinant matrix of order $4k + 1$ by adjoining an additional row and column.

To optimize our method in a given dimension, we seek a 3-normalized Hadamard “starting” matrix whose excess, defined as the sum of all matrix entries (see Definition 2.3), is as large as possible. In §4, we derive an upper bound on this excess. The determinants attainable by the maximal excess construction are also bounded, given the bounds on the excess of an Hadamard matrix first noted by Brown & Spencer [BS], and later improved by Kounias & Farmakis [KF]. Comparison of the analogous bounds suggests that our method has the potential to construct determinants larger than any obtainable using the maximal excess method in arbitrarily high dimensions.

Furthermore, for $n$ up to about 100, we find Hadamard matrices that attain or closely approach our bound, thus establishing the records mentioned above. On the other hand, we do not yet know of any infinite family of Hadamard matrices that attains our bound, while several such families are known for the maximal excess construction. We should also note that asymptotically, the largest fraction of Barba’s bound that either method can attain is $B(n)/\sqrt{2} \approx 0.71B(n)$. Our bound does exceed that of Kounias & Farmakis by a lower order term as $n \to \infty$, however, as shown in Proposition 4.4.

2. Preliminaries

Maximal determinants. Let $\{\pm 1\}^{n \times n}$ denote the space of all $n \times n$ sign matrices—matrices populated entirely by $\pm 1$s. This space has cardinality $2^{n^2} < \infty$, so for each $n \in \mathbb{Z}$, there exists a sign matrix of maximal determinant. Define the maximal determinant function accordingly:

$$\text{md} : |\mathbb{Z}| \to |\mathbb{Z}|, \quad \text{md}(n) := \max \{\det A : A \in \{\pm 1\}^{n \times n}\}.$$


The exact value of $\text{md}(n)$ has been established for all $n \leq 26$ except $n = 19, 22$ and 23. An elementary argument first given by Hadamard shows that we always have $\text{md}(n) \leq \frac{n^n}{2}$, with equality iff the maximizing matrix is Hadamard, i.e. a sign matrix with mutually orthogonal rows. A well-known conjecture states that Hadamard matrices of order $n$ exist for all $n \equiv 0 \pmod{4}$, so that the bound is achieved in these dimensions. This conjecture is known to hold for all $n \equiv 0 \pmod{4}$ with $n < 428$, and many larger values as well [SY].

The present paper focuses entirely on the case $n \equiv 1 \pmod{4}$, for which $\text{md}(n)$ remains largely unknown. For $n \geq 29$ with $n \equiv 1 \pmod{4}$, we only know $\text{md}(n)$ when $n$ takes the form $a^2 + (a + 1)^2$ when $a$ is an odd prime power [HH], and when $a = 4$ [BHH]. For these values of $n$, as well as $n = 1, 5, 13, \text{and} 25$, the maximizing matrix is essentially the incidence matrix of a suitable block design, and $\text{md}(n)$ attains the upper bound $B(n)$ for odd $n$ given in [11] above. Conversely, equality cannot hold here unless $n = a^2 + (a + 1)^2$ for some integer $a$, which forces $n \equiv 1 \pmod{4}$. Conjecturally, Barba’s bound is attained whenever $n$ has this form.

Tensor notation. Given vectors $x, y \in \mathbb{R}^n$ with coordinates $x_i, y_j$, we will identify the tensor product $x \otimes y$ with the rank-1 linear transformation whose action on $\mathbb{R}^n$ and matrix entries $[x \otimes y]_{ij}$ are characterized respectively by

\begin{equation}
(x \otimes y)(v) := (y \cdot v)x, \quad [x \otimes y]_{ij} = x_iy_j.
\end{equation}

For any $A \in \text{Hom}(\mathbb{R}^n)$, we then have

\begin{equation}
A \circ (x \otimes y) = (Ax) \otimes y, \quad \text{and} \quad (x \otimes y) \circ A = x \otimes (t^A y),
\end{equation}

where $t^A$ denotes the transpose of $A$. In particular, when $A = c \otimes d$ for some $c, d \in \mathbb{R}^n$, we have

\begin{equation}
(x \otimes y) \circ (c \otimes d) = (y \cdot c)x \otimes d.
\end{equation}

Note also that

\begin{equation}
t^A(x \otimes y) = y \otimes x.
\end{equation}

Using these facts, we get well-known formulae for the inverse and determinant of the “rank-1 update” of a non-singular matrix:

**Lemma 2.1** (Sherman-Morrison formulae). If $x, y \in \mathbb{R}^n$ and $A_{n \times n}$ is invertible, then

\[
\begin{align*}
\text{det}(A + x \otimes y) &= (\text{det} A) (1 + A^{-1}x \cdot y) \\
(A + x \otimes y)^{-1} &= A^{-1} - \frac{A^{-1}x \otimes (t^A y)}{1 + A^{-1}x \cdot y}
\end{align*}
\]
Proof. First consider the special case $A = I_n$, and choose an orthonormal basis $\{\tilde{e}_j\}$ for $\mathbb{R}^n$ with $\tilde{e}_1 = x/|x|$. Then

$$(x \otimes y)(\tilde{e}_j) = (y \cdot \tilde{e}_j)x = (y \cdot \tilde{e}_j)|x|\tilde{e}_1,$$

It follows that, relative to this basis, the matrix representing $I_n + x \otimes y$ has zeros everywhere except along the first row, and the diagonal. In particular, it is upper triangular, with all diagonal entries equal to 1 except the first, which is $1 + x \cdot y$. The determinant of $I_n + x \otimes y$ then reduces to this single entry, and we then have, for any invertible $n \times n$ matrix $A$,

$$\det(A + x \otimes y) = (\det A) \det (I_n + A^{-1}(x \otimes y)) = (\det A) \det (I_n + (A^{-1}x) \otimes y) = (\det A) (1 + A^{-1}x \cdot y).$$

This gives the stated formula for determinants.

One can verify the formula for the inverse directly: Multiply it on the right by $(A_x \otimes y)$, and simplify, using the rules in \[2\] The result, a straightforward calculation, is $I_n$. □

Definition 2.2. To streamline the display of vectors and matrices below, we introduce the following convention: Given any integer $n$, and any $k \in \mathbb{Z}$, $n_k := n(1, 1, \ldots, 1) \in \mathbb{R}^k$. Abusing notation slightly, we also use $n_i$ to indicate a sequence of $k$ copies of the number $n$. For instance,

$$(3_{11}, -1_9) = (3, \underline{3}, \ldots, 3, -1, -1, \ldots, -1) \in \mathbb{R}^{20}.$$

Excess. If $A \in \{\pm 1\}^{n \times n}$, then the sum of the entries of $A$ measures the extent to which the +1s “exceed” the number of −1s in $A$.

Definition 2.3 (Excess and row sums). The excess of any vector or matrix $X$ is the sum of its entries, and we denote it by $\text{ex} (X)$. Note that for a vector $x \in \mathbb{R}^k$ or an $n \times m$ matrix $A$ respectively, we have

$$\text{(7)} \quad \text{ex} (x) := x \cdot 1_k, \quad \text{ex} (A) := 1_n \cdot A 1_m.$$

We call the excess of the $i$th row of a matrix its $i$th row sum.

Observation 2.4. If $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$, then

$$\text{ex} (x \otimes y) = \text{ex} (x) \text{ ex} (y).$$

This follows immediately from \[3\].
The injection $E : \mathbb{R}^{n \times n} \to \mathbb{R}^{(n+1) \times (n+1)}$. Let $\mathbb{R}^{n \times n}$ denote the space of all real $n \times n$ matrices. Several of the facts above come together in relation to the map $E : \mathbb{R}^{n \times n} \to \mathbb{R}^{(n+1) \times (n+1)}$, which adds an additional first row and column to $A$ by prepending $-1$ to each row of $A$, and then prepends an entire row of $+1$s to that. In block form, we may express this as follows:

$$E(A_{n \times n}) := \begin{pmatrix} 1 & 1_n \\ -1_n & A \end{pmatrix}.$$  

Lemma 2.5. For any square matrix $A$, we have

$$\det(E(A)) = (\det A) \left(1 + \exp(A^{-1})\right).$$

Proof. Adding the first row of $E(A)$ to each successive row produces the matrix

$$\begin{pmatrix} 1 & 1_n \\ 0_n & A + 1_n \otimes 1_n \end{pmatrix},$$

without changing the determinant. The determinant of the latter matrix is simply the determinant of its lower-right block, however. We thus have

$$\det(E(A)) = \det(A + 1_n \otimes 1_n).$$

The desired result now follows immediately from Lemma 2.1 and (7). \qed

Hadamard matrices. As mentioned above, a Hadamard matrix is an element $H \in \{-1,1\}^{n \times n}$ whose rows are mutually orthogonal. We denote the set of $n \times n$ Hadamard matrices by $\text{Had}(n)$.

Row and column permutations, and row and column negations, clearly leave $\text{Had}(n)$ invariant. Hence

Definition 2.6. Hadamard matrices $H_1, H_2 \in \text{Had}(n)$ are equivalent if $H_1$ can be transformed into $H_2$ by permuting and/or negating sets of rows and/or columns.

We also note here that $\text{Had}(n) \subset \{-1,1\}^{n \times n}$ is invariant under transposition. Indeed, the defining condition for $H \in \text{Had}(n)$ implies that $H^tH = n I_n$, and hence that $H^{-1} = \frac{1}{n} H^t$. 

Proposition 2.7. If $n > 2$ and $H \in \text{Had}(n)$, then $n = 4k$ for some $k \in \mathbb{Z}^+$, and using only column swaps and column negations, we can put the first 3 rows of $H$ into the following standard form

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


Here ‘+’ and ‘−’ respectively abbreviate $+1_k$ and $-1_k$. Moreover, if we denote the $i$th row sum of $H$ by $r_i$, we have

$$\sum_{i=1}^{4k} r_i^2 = 16k^2.$$  

**Proof.** To begin, note that by negating column $j$ of $H = [h_{ij}]$ whenever $h_{1j} = -1$, we get an equivalent matrix whose first row contains only $+1$’s. If we then sort the columns of the resulting matrix in decreasing lexicographic order, left to right, the first three rows of the resulting $H$-equivalent matrix will necessarily take the form

$$\begin{pmatrix} +1_{k_1} & +1_{k_2} & +1_{k_3} & +1_{k_4} \\ +1_{k_1} & +1_{k_2} & -1_{k_3} & -1_{k_4} \\ +1_{k_1} & -1_{k_2} & +1_{k_3} & -1_{k_4} \end{pmatrix},$$

where $k_1 + k_2 + k_3 + k_4 = n$, and the mutual orthogonality of these rows gives three additional equations:

$$k_1 + k_2 - k_3 - k_4 = 0$$
$$k_1 - k_2 + k_3 - k_4 = 0$$
$$k_1 - k_2 - k_3 + k_4 = 0$$

The unique solution of the resulting $4 \times 4$ system is $k_1 = k_2 = k_3 = k_4 = n/4$, and since each $k_i$ is an integer, we have $n/4 \in \mathbb{Z}^+$. This proves the first two claims.

To get the fact about row sums, note that the the vector $(r_1, r_2, \ldots, r_{4k})$ of row sums coincides with $H1_{4k}$. It follows that

$$\sum_{i=1}^{4k} r_i^2 = H1_{4k} \cdot H1_{4k} = 1_{4k} \cdot (HH)1_{4k} = 1_{4k} \cdot (4k1_{4k}) = (4k)^2.$$

This completes the proof. \qed

Though the first three rows of any Hadamard matrix can always be put in the form (9), a different normalization will better suit our purposes.

**Definition 2.8** (3-normalization). When the first three rows of a Hadamard matrix $H$ have the form

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

and all row sums of $H$ are non-negative, we say that $H$ is 3-normalized.
Proposition 2.9. Every Hadamard matrix $H \in \text{Had}(n)$, $n > 2$, can be 3-normalized using column swaps, column-negation, and row-negation only. Moreover, every 3-normalized Hadamard matrix has the form

$$N = \begin{pmatrix}
  + & - & - & + \\
  + & - & + & - \\
  + & + & - & - \\
  a_1 & b_1 & c_1 & d_1 \\
  \vdots & \vdots & \vdots & \vdots \\
  a_n & b_n & c_n & d_n
\end{pmatrix}.$$  

Here ‘+’ and ‘−’ respectively abbreviate $\pm 1_k$, and $a_i, b_i, c_i, d_i \in \{\pm 1\}^{n/4}$, and satisfy, for each $i = 4, \ldots, n$,

$$\text{ex}(a_i) = \text{ex}(b_i) = \text{ex}(c_i) = \text{ex}(d_i).$$

For the row sums $r_i$, we have $r_1 = r_2 = r_3 = 0$, and, for $i > 3$, $r_i \equiv n \pmod{8}$. If $n \equiv 4 \pmod{8}$, $r_i \leq n - 8$ for all rows, unless $n = 4$.

Finally, we have $\text{ex}(N) \equiv n \pmod{8}$, and when $n \equiv 0 \pmod{8}$, $\text{ex}(N) \equiv n \pmod{16}$.

Proof. By Proposition 2.7, we can write $n = 4k$ and put the first three rows of $H$ into the form (9) using only column swaps and negations. By further negating columns $k + 1$ through $3k$, we obtain an $H$-equivalent matrix whose first three rows have the form (11). Negating all rows having negative row sums, we now get a 3-normalized Hadamard matrix equivalent to $H$. This proves the Lemma’s first statement.

To get (12), define $a_i = \text{ex}(a_i)$, $b_i = \text{ex}(b_i)$, etc., and recall that for any fixed $i = 4, 5, \ldots, n$, row $i$ is orthogonal to each of the first three rows. Consequently,

$$a_i - b_i - c_i + d_i = 0$$
$$a_i - b_i + c_i - d_i = 0$$
$$a_i + b_i - c_i - d_i = 0.$$

The general solution here is $a_i = b_i = c_i = d_i$, which proves (12). It also shows that $r_i \equiv 0 \pmod{4}$ for all $i$. In fact, the first three row sums clearly equal 0, and to get the more precise claim about rows 4 through $n$, simply note that since $a_i$ has $k$ entries, each congruent to 1 mod 2, $\text{ex}(a_i)$ has the same parity as $k$ does.

It follows that $r_i = 4\text{ex}(a_i) \equiv 0$ or 4 (mod 8), depending on whether $k$ is even or odd respectively.

For odd $k > 1$, no row can consist entirely of 1s (giving row sum $n$), because the mutual orthogonality of rows would then force all remaining row sums to equal $0 \not\equiv 4 \pmod{8}$. Therefore, no row sum exceeds $n - 8$ in this case, as claimed.
Since we have an odd number \((n - 3)\) of non-zero row sums, all congruent to \(n \mod 8\), it follows that \(\text{ex}(N) \equiv n \mod 8\).

Finally, since \(r_i \equiv n \mod 8\), we may write \(r_i = 8l_i\) and \(n = 8m\) when \(n \equiv 0 \mod 8\). By definition of the excess, and (10) above, we then have

\[
\frac{\text{ex}(N)}{8} = \sum_{i=1}^{n} l_i \quad \text{and} \quad m^2 = \sum_{i=1}^{n} l_i^2.
\]

Since \(x^2 \equiv x \mod 2\) for any integer \(x\), the two sums above, and \(m\), all have the same parity. We conclude that \(\text{ex}(N) \equiv 8m \mod 16\), as claimed.

\(\Box\)

\textbf{Remark 2.10.} When \(n \geq 20\) and \(n \equiv 4 \mod 8\), the proof of Lemma 2.2 in [Ha] generalizes to show that the largest possible row sum allowed by Proposition 2.9 above, namely \(n - 8\), can be achieved by at most one row. Modulo column negations and permutations, such a row forms, along with the three initial rows of the 3-normalized matrix to which it belongs, a Hall set, as defined by Kimura [Ki].

\section*{3. A Construction}

\textbf{Constructing} \(\Gamma(N)\). We now describe the basic construction we use to produce large-determinant sign matrices of order \(n+1\).

\begin{enumerate}
\item \textbf{Step 1:} Select a 3-normalized Hadamard matrix \(N \in \text{Had}(n)\), \(n = 4k\).
\item \textbf{Step 2:} Alter \(N\) by negating its first \(k\) columns to produce a new Hadamard matrix \(N'\). By Lemma 2.9 the first three rows of \(N'\) will take the form

\[
\begin{pmatrix}
- & - & - & + \\
- & - & + & - \\
- & + & - & - \\
\end{pmatrix}.
\]

\item \textbf{Step 3:} Make the rank-1 modification

\[
N' \rightarrow N' + 2\epsilon_3 \otimes \epsilon_k =: N'',
\]

where, for any \(m \in |\mathbb{Z}|\) we define \(\epsilon_m := (1_m, 0_{n-m}) \in \mathbb{R}^n\). This modifies \(N'\) by changing the \(-1\)s in its upper left \(3 \times k\) block to \(+1\)s. Note also that \(N''\) is no longer Hadamard.

\item \textbf{Step 4:} Construct the final sign matrix \(\Gamma(N)\) of size \(n+1\) by applying the injection \(E\) defined in [2]

\[
\Gamma(N) = E(N'').
\]
\end{enumerate}

The following result suggests the efficacy of this construction.
Theorem 3.1. Let $N$ be a 3-normalized Hadamard matrix of order $n = 4k$. Then the sign matrix $\Gamma(N)$ of order $n + 1$ described above has determinant

$$\det \Gamma(N) = (\det N) \left( 2 + \frac{\text{ex}(N)}{n} \right) = \pm n^{n/2} \left( 2 + \frac{\text{ex}(N)}{n} \right).$$

Proof. Using the notation of our construction above, we can express $\det \Gamma(N)$ in terms of $N''$ by applying Lemma 2.5 to get:

$$\text{(14)} \quad \det \Gamma(N) = \det N'' \left( 1 + \text{ex} \left( N''^{-1} \right) \right).$$

We proceed to expand the right-hand side in terms of $N$ itself. First, given the definition of $N''$ in Step 3 of our construction, Lemma 2.1 enables us to write

$$\text{(15)} \quad \det N'' = (\det N') \left( 1 + 2 N'^{-1} \epsilon_3 \cdot \epsilon_k \right).$$

Since $N'$ is Hadamard, we have $N'^{-1} = tN'/n$, and hence $N'^{-1} \epsilon_3 = tN' \epsilon_3/n$. But $tN' \epsilon_3$ simply sums the the first three columns of $tN'$, i.e. the first three rows of $N'$ itself. Step 2 of our construction displays these rows explicitly, and we easily deduce

$$\text{(16)} \quad N'^{-1} \epsilon_3 = \frac{1}{n} \left( -3_k, -1_{3k} \right).$$

It follows that

$$\text{(17)} \quad 1 + 2 N'^{-1} \epsilon_3 \cdot \epsilon_k = 1 + \frac{2}{n} \begin{pmatrix} -3_k \\ -1_{3k} \end{pmatrix} \cdot \begin{pmatrix} 1_k \\ 0_{3k} \end{pmatrix} = 1 - \frac{2}{n} \cdot 3k = -\frac{1}{2},$$

and consequently,

$$\text{(18)} \quad \det N'' = (-1)^{k+1} \frac{\det N}{2}.$$ 

The factor $(-1)^k$ appears because we have replaced $N'$ by $N$, a matter of negating $k$ columns.

We next calculate $\text{ex}(N'^{-1})$.

To begin, invert $N'' = N' + 2 \epsilon_3 \otimes \epsilon_k$ using Lemma 2.1 and compute

$$\text{ex}(N'^{-1}) = \text{ex}(N'^{-1}) - 2 \frac{\text{ex}(N'^{-1} \epsilon_3 \otimes (tN')^{-1} \epsilon_k)}{1 + 2 N'^{-1} \epsilon_3 \cdot \epsilon_k}$$

$$= \text{ex}(N'^{-1}) + 4 \text{ex}(N'^{-1} \epsilon_3) \cdot \text{ex} \left( (tN')^{-1} \epsilon_k \right).$$

Here we used (17) to evaluate the denominator, and Observation 2.1 to factor the excess of the tensor product.
Now unpack the excess terms on the right above. For \( i = 1, 2, \ldots, n \), let \( r_i \) and \( r'_i \) denote the \( i \)th row sums of \( N \) and \( N' \) respectively. Since \( N' \) is Hadamard, we may then write

\[
\text{ex} \left( N'^{-1} \right) = \frac{1}{n} \text{ex} \left( N' \right) = \frac{1}{n} \sum_{i=1}^{n} r'_i .
\]

We obtained \( N' \) from a 3-normalized Hadamard matrix \( N \) by negating columns \( 1 \) through \( k \). So by the definition of 3-normalized form, we have \( r'_i = -2k = -n/2 \) when \( i = 1, 2, 3 \). When \( i \geq 4 \) Proposition 2.9 similarly implies \( r'_i = r_i / 2 \). Finally, since \( r_1 = r_2 = r_3 = 0 \), we have

\[
\sum_{i=1}^{n} r_i = \sum_{i=1}^{n} r'_i = \text{ex} \left( N \right) .
\]

Thus

\[
(20) \quad \text{ex} \left( N'^{-1} \right) = \frac{1}{n} \cdot \left( \sum_{i=1}^{3} r'_i + \sum_{i=4}^{n} r'_i \right) = \frac{1}{n} \cdot \left( -3n + \text{ex} \left( N \right) \right) = \frac{\text{ex} \left( N \right) - 3}{2} .
\]

Given these facts, we now easily analyze \( \text{ex} \left( N'^{-1}_3 \right) \) using (16):

\[
(21) \quad \text{ex} \left( N'^{-1}_3 \right) = \frac{1}{n} \left( -3 \cdot \frac{n}{4} + (-1) \cdot \frac{3n}{4} \right) = -\frac{6}{4} = -\frac{3}{2} .
\]

Lastly, we compute \( \text{ex} \left( (N')^{-1}_k \epsilon_k \right) \), recalling again that we produce \( N' \) from \( N \in \text{Had} \left( n \right) \) by negating columns 1 through \( k \), so that

\[
\left( N' \right)^{-1}_k = \frac{1}{n} N' \epsilon_k = \frac{1}{n} \cdot \left( \text{sum of the first } k \text{ columns of } N' \right) = \frac{1}{n} \cdot \left( \text{sum of the first } k \text{ columns of } N \right) .
\]

Since \( N \) is 3-normalized, rows 1, 2, and 3 have only +1s in these columns. The first three rows therefore contribute \( k = n/4 \) each to the sum of columns above. Proposition 2.9 further guarantees that rows 4 through \( n \) each contribute exactly 1/4th of their full row sum. Denoting the latter row sums by \( r_i \) as above, we may therefore write

\[
\left( N' \right)^{-1}_k = -\frac{1}{4n} \left( n_3, r_4, r_5, \ldots, r_n \right) ,
\]

whence

\[
(22) \quad \text{ex} \left( (N')^{-1}_k \epsilon_k \right) = -\frac{1}{4n} \left( 3n + \text{ex} \left( N \right) \right) = -\frac{\text{ex} \left( N \right)}{4n} - \frac{3}{4} ,
\]

since \( \sum_{i=4}^{n} r_i = \text{ex} \left( N \right) \), as noted in deriving (20) above.

Finally, we assemble the various facts above to calculate \( \det \Gamma \left( N \right) \). First, combine equations (14), (18) and (19), to get

\[
\det \Gamma \left( N \right) = (-1)^{k+1} \left( \det N \right) \cdot \frac{1}{2} \cdot \left( 1 + \text{ex} \left( N'^{-1} \right) + 4 \text{ex} \left( N'^{-1}_3 \right) \cdot \text{ex} \left( (N')^{-1}_k \epsilon_k \right) \right) .
\]

Then replace the excess terms here with the results of equations (20), (21), and (22). Routine simplification then verifies the theorem. \( \square \)
4. Upper bounds

Compare the formula in Theorem 3.1 above with the analogous formula we get by applying Lemma 2.5 to an arbitrary $n \times n$ Hadamard matrix $H$:

$$\det (E(H)) = (\det H) \left( 1 + \frac{1}{n} \text{ex}(H) \right).$$

The latter formula clearly shows that we maximize $\det E(H)$ over all $H \in \text{Had}(n)$ by maximizing $\text{ex}(H)$. Indeed, this constitutes the maximal excess technique of Farmakis & Kounias [FK] we mention in our introduction.

By comparison, Theorem 3.1 above shows that we can improve on that technique in any dimension $n$ where there exists a 3-normalized $n \times n$ Hadamard matrix $N$ such that

$$\text{ex}(N) + n > \text{ex}(H) \quad \text{for all } H \in \text{Had}(n).$$

Of course, the 3-normalized matrices form a relatively small subset in any equivalence class of Hadamard matrices, and one expects the excess function to reach a smaller max on this subset than on the entire class. So it is not obvious that we can attain the desirable situation expressed by (24).

We have found, however, that 3-normalized Hadamard matrices satisfying (24) do exist, at least in dimensions $n < 100$. The excesses of arbitrary Hadamard matrices and 3-normalized Hadamard matrices satisfy certain natural upper bounds. We discuss both bounds below, and compare them. We find that for large $n$, the bounds themselves do satisfy (24), offering the hope that one could find an actual 3-normalized matrix that does so.

In this section, we briefly review known bounds on the excess of a general Hadamard matrix $H \in \text{Had}(n)$, then derive a new upper bound for the excess of a 3-normalized Hadamard matrix. Our bound clarifies what we can (and cannot) hope to obtain from the construction in §3 and indicates how to optimize the search for suitable 3-normalized Hadamard matrices, which we take up in §5.

Proposition 4.4 at the end of this section gives our comparison of the two bounds.

The $n^{3/2}$ bound on maximal excess. The excess of a general Hadamard matrix $H \in \text{Had}(n)$ can never exceed $n^{3/2}$. Indeed, the Cauchy-Schwartz inequality gives

$$\text{ex}(H) = 1_n \cdot H1_n \leq |1_n| \cdot |H1_n| = \sqrt{n} \cdot \sqrt{n} \cdot \sqrt{n},$$

since $H/\sqrt{n}$ is orthogonal. This fact was apparently first observed by Brown & Spencer [BS], and independently, by Best [Be]. The bound is sharp in the sense that regular Hadamard matrices actually attain this excess value, and such matrices occur in infinitely many orders (for instance, order $n^2$ whenever $\text{Had}(n)$ is non-empty [CS]).
In [KF], Kounias & Farmakis derive an upper bound smaller than $n^{3/2}$ when $n$ is not a perfect square, and tabulate their bound versus the largest known excess for all orders up to $n = 100$ [FK]. For convenience, we reproduce their list of bounds in Table 1, §5.

A 3-normalized excess bound. If $N$ is a 3-normalized Hadamard matrix of order $n > 2$, Prop. [2.9] shows that the first three rows of $N$ have row sum zero, while the remaining row sums belong to the set

$$\text{RS}(n) = \begin{cases} \{0, 8, 16, \ldots, n\}, & \text{if } n \equiv 0 \pmod{8}, \\ \{4\}, & \text{if } n = 4, \\ \{4, 12, 20, \ldots, n-8\}, & \text{if } n \equiv 4 \pmod{8}, n > 4. \end{cases}$$

**Observation 4.1.** Consider the last $n-3$ rows of a 3-normalized $N \in \text{Had}(n)$. For each $r \in \text{RS}(n)$, let $n_r$ count how many of these rows have row sum $r$. Then

$$\sum_{\text{RS}(n)} n_r = n-3, \quad \sum_{\text{RS}(n)} r n_r = \text{ex}(N), \quad \text{and} \quad \sum_{\text{RS}(n)} r^2 n_r = n^2.$$

**Proof.** The first identity is trivial. The second totals the row sums—the excesses—of the last $n-3$ rows. Since the first three rows of $N$ contribute zero excess, this gives $\text{ex}(N)$. Equation (10) from Prop. 2.7 evaluates the third sum; we record it in slightly different notation here for convenience only. □

**Notation.** In the theorem below, the notations

$$[x] \quad \text{and} \quad [x]_+$$

respectively denote the ceiling and positive ceiling of $x$, i.e. least integer, and the least positive integer, respectively, which exceeds or equals $x$.

**Theorem 4.2.** Suppose $N \in \text{Had}(n)$ is 3-normalized, with $n \geq 4$. Then $\text{ex}(N) \leq \nu^*_n$, where

$$\nu^*_n := \frac{\bar{\rho}_n(n-3)}{2} + \frac{(n-4)(n-12)}{2\bar{\rho}_n}, \quad (25)$$

and

$$\bar{\rho}_n := \begin{cases} 8 \left\lfloor \frac{n}{8\sqrt{n-3}} \right\rfloor - 4, & \text{if } n \equiv 0 \pmod{8}, \\ 8 \left\lfloor \frac{n}{8\sqrt{n-3}} - \frac{1}{2} \right\rfloor + 1, & \text{if } n \equiv 4 \pmod{8}. \end{cases}$$

Equality holds in (25) iff the last $n-3$ row sums of $N$ take the values $\bar{\rho}_n \pm 4$ only.

**Proof.** Our main argument degenerates for the cases $n = 4, 8$ and 12; we consequently argue the latter separately after handling the generic case $n > 12$. 
The case $n > 12$. As in Observation 4.1, we let $n_r$ count how many, among the last $n - 3$ rows of $N$, have row sum $r$ for each $r \in \text{RS}(n)$. We then adapt a technique appearing in Kounias and Farmakis [KF] by considering the following function $F$ of $\rho \in \text{RS}(n)$:

$$F(\rho) := \sum_{\text{RS}(n)} n_r(\rho - r)(\rho + 8 - r) \geq 0.$$  

The inequality here is crucial. It holds because the $n_r$ are all non-negative, while $(\rho - r)$ and $(\rho + 8 - r)$ necessarily give consecutive integer multiples of 8, and hence a non-negative product.

On the other hand, $F(\rho)$ expands as

$$F(\rho) = \rho(\rho + 8) \sum n_r - (2\rho + 8) \sum r n_r + \sum r^2 n_r,$$

and we can evaluate all three sums explicitly using Observation 4.1. After careful simplification, we may then rewrite the estimate (26) above as

$$\text{ex}(N) \leq G_n(\rho) := \frac{(\rho + 4)(n - 3)}{2} + \frac{(n - 4)(n - 12)}{2(\rho + 4)}.$$  

Note too, for later use, that equality obtains here iff $F(\rho) = 0$.

To extract the strongest possible result from (27), we now minimize $G_n(\rho)$ over RS $(n)$. Here, the assumption $n > 12$ comes into play; one easily sees that in this case $G_n$ is concave up, hence attains its minimum on RS $(n)$ at the smallest $\rho \in \text{RS}(n)$ for which the forward difference $G_n(\rho + 8) - G_n(\rho)$ is non-negative. Accordingly, we compute

$$G_n(\rho + 8) - G_n(\rho) = 4 \left(\frac{(\rho + 8)^2(n - 3) - n^2}{(\rho + 4)(\rho + 12)}\right),$$

and observe that the denominator here is positive for all $\rho \in \text{RS}(n)$. This makes non-negativity of the forward difference on RS $(n)$ equivalent to

$$\rho \geq \frac{n}{\sqrt{n - 3}} - 8.$$  

Since RS $(n)$ depends on the residue class of $n \mod 8$, so does the minimal solution $\rho_{\text{min}} \in \text{RS}(n)$ for this inequality, but a little thought shows that we can express it in the following way:

$$\rho_{\text{min}} = \begin{cases} 8 \left[\frac{n}{8\sqrt{n - 3}}\right] - 8, & \text{if } n \equiv 0 \pmod{8} \\ 8 \left[\frac{n}{8\sqrt{n - 3}} - \frac{1}{2}\right] - 4, & \text{if } n \equiv 4 \pmod{8}. \end{cases}$$  

By evaluating (27) with $\rho = \rho_{\text{min}}$ and then substituting $\bar{\rho}_n := \rho_{\text{min}} + 4$, we now obtain (25), the main result of our theorem.
It remains to analyze the condition for equality there. According to the remark immediately following (27), this condition corresponds to \( F(\rho_{\text{min}}) = 0 \), and by (26), the latter will happen if and only if we have

\[
n_r(\rho_{\text{min}} - r)(\rho_{\text{min}} + 8 - r) = 0 \quad \text{for all } r \in \text{RS}(n).
\]

The factor \((\rho_{\text{min}} - r)(\rho_{\text{min}} + 8 - r)\) here vanishes when and only when \( r = \rho_{\text{min}} \) or \( r = \rho_{\text{min}} + 8 \), or equivalently, when \( r = \bar{\rho}_n \pm 4 \). Equality in (25) consequently forces \( n_r = 0 \) for all other \( r \in \text{RS}(n) \), exactly as claimed.

**The cases ** \( n = 4, 8 \text{ and } 12 \). Since \( \text{RS}(4) = \text{RS}(12) = \{4\} \), the excess of a 3-normalized Hadamard matrix \( N \) will equal \((4 - 3) \times 4 = 4 \) if \( N \in \text{Had}(4) \), and \((12 - 3) \times 4 = 36 \) if \( N \in \text{Had}(12) \). The reader will easily check that our theorem accurately predicts these values and appropriately assigns \( \bar{\rho}_n = 8 \).

When \( n = 8 \), we have \( \text{RS}(8) = \{0, 8\} \). In fact, a 3-normalized matrix \( N \in \text{Had}(8) \) will have exactly one row with sum 8 and seven with row sum 0. For, on the one hand, all eight rows cannot sum to zero; this would make them linearly dependent. On the other hand, all entries in a row with sum 8 must be +1s, so even two such rows create a dependency. We consequently have \( \text{ex}(N) = 8 \), again confirming the theorem. \( \square \)

**Remark 4.3.** According to Prop. 2.9 the excess of a 3-normalized matrix \( N \in \text{Had}(n) \) always has certain congruence properties. The bound \( \nu_n^* \) in Theorem 4.2 however, may not have these properties, and in such cases, we cannot achieve \( \text{ex}(N) = \nu_n^* \). This occurs for the first time, for instance when \( n = 80 \equiv 0 \pmod{16} \).

Then \( \bar{\rho}_n = 12 \) and \( \nu_n^* = 6771/3 \). By Proposition 2.9 however, the excess of any actual 3-normalized \( N \in \text{Had}(80) \) must be divisible by 16. Since the largest multiple of 16 below \( \nu_{80}^* \) is 672, the latter provides a sharper upper bound for \( \text{ex}(N) \) when \( n = 80 \). We know no 3-normalized \( N \in \text{Had}(80) \) with excess above 624, but if there exists a matrix \( N \in \text{Had}(80) \) with \( n_0 = 1 \) (ie. 1 row with excess 0), \( n_8 = 68 \) and \( n_{16} = 8 \), it has excess 672, thus attaining the sharper bound.

In general, when this situation arises (the next such occurs when \( n = 104 \) ), our bound can be sharpened similarly. The precise formulation, using \( \lfloor x \rfloor \) to denote the integer part of \( x \) is as follows:

\[
\text{ex}(N) \leq \begin{cases} 
8 \left\lfloor \frac{\nu_n^*}{8} - \frac{1}{2} \right\rfloor + 4 & \text{if } n \equiv 4 \pmod{8}, \\
16 \left\lfloor \frac{\nu_n^*}{16} - \frac{1}{2} \right\rfloor + 8 & \text{if } n \equiv 8 \pmod{16}, \\
16 \left\lfloor \frac{\nu_n^*}{16} \right\rfloor & \text{if } n \equiv 0 \pmod{16}.
\end{cases}
\]
We should emphasize, however, that even this sharpened bound may not be attained for all \( n \). Indeed, it remains unknown whether \( \text{Had}(n) \) is non-empty for all \( n \equiv 0 \pmod{4} \).

**Comparison of bounds.** As discussed at the beginning of this section, our construction (Theorem 3.1) produces a determinant larger than any the maximal excess method can construct whenever there exists a 3-normalized Hadamard matrix \( N \in \text{Had}(n) \) for which (24) holds. Given the \( n^{3/2} \) bound on maximal excess, (24) certainly holds whenever

\[
\text{ex}(N) + n > n^{3/2}.
\]

We now show that Theorem 4.2 presents no obstruction to the existence of such a matrix \( N \), except in the very lowest dimensions. Recall that \( \nu^*_n \), defined in that theorem, denotes our upper bound for the excess of a 3-normalized Hadamard matrix in \( \text{Had}(n) \).

**Proposition 4.4.** For all \( n \geq 12 \) we have

\[
\sqrt{(n-3)(n-4)(n-12)} \leq \nu^*_n \leq n\sqrt{n-3},
\]

so that \( \nu^*_n = n^{3/2} - O(\sqrt{n}) \), and \( (\nu^*_n + n) - n^{3/2} \sim n \) as \( n \to \infty \) in the sense that

\[
\lim_{n \to \infty} \frac{(\nu^*_n + n) - n^{3/2}}{n} = 1.
\]

In fact, for all \( n \geq 88 \), we have

\[
\nu^*_n + n > n^{3/2},
\]

**Proof.** It is clear from the definition of \( \nu^*_n \) (and that fact that \( \bar{\rho}_n > 0 \)) that we can bound \( \nu^*_n \) from below by the minimum of the function

\[
G_n(x) = \frac{(n-3)x}{2} + \frac{(n-4)(n-12)}{2x}, \quad x \in (0,\infty).
\]

(We minimized essentially the same function in proving Theorem 4.2 but over a discrete domain.)

When \( n > 12 \), the function is concave up, with one critical point on \((0,\infty)\). Computing the minimum explicitly on this interval, one easily obtains the lower bound in (29) when \( n > 12 \). The bound is trivial when \( n = 12 \).

To get the upper bound \( \nu^*_n < n\sqrt{n-3} \), we note that the definition of \( \bar{\rho}_n \) also implies

\[
\frac{n}{\sqrt{n-3}} + 4 \geq \bar{\rho}_n \geq \frac{n}{\sqrt{n-3}} - 4.
\]

If we restrict \( x \) to this interval, the maximum of \( G_n(x) \) must occur at an endpoint, and an easy calculation shows that \( G_n(x) = n\sqrt{n-3} \) at both endpoints. This value consequently bounds \( \nu^*_n \) from above, as claimed.
The asymptotic result \( \nu_n^* = n^{3/2} - O(\sqrt{n}) \) now follows. In fact, one easily uses the bounds in (29) to compute

\[
-\frac{3}{2} \geq \limsup_{n \to +\infty} \frac{\nu_n^* - n^{3/2}}{\sqrt{n}} \geq \liminf_{n \to +\infty} \frac{\nu_n^* - n^{3/2}}{\sqrt{n}} \geq -\frac{19}{2}.
\]

These facts make (30) obvious, and imply that (31) holds for sufficiently large \( n \).

To show more precisely that (31) holds whenever \( n \geq 88 \), it will suffice to do so with \( \nu_n^* \) replaced by the lower bound in (29); that is to show

\[
(\sqrt{n} - 3)(\sqrt{n} - 4)(\sqrt{n} - 12) > n^{3/2} - n \quad \text{for all } n \geq 88.
\]

Squaring both sides and simplifying the result we find that this inequality is equivalent to

\[
(n^{5/2} - 10n^2) + (48n - 72) > 0.
\]

When \( \sqrt{n} > 10 \), the first term in parentheses here is clearly non-negative, and the second is positive. We therefore see that (31) holds for all \( n \geq 100 \). By hand, one checks that it holds for \( n = 96, 92 \) and 88 as well, but not for \( n = 84 \).

As mentioned earlier, Kounias & Farmakis bound the maximal excess of an order-\( n \) Hadamard by a number \( \sigma_n^* < n^{3/2} \) when \( n \) is not a perfect square. For \( n < 88 \), our bound \( \nu_n^* + n \) dips below \( n^{3/2} \), but it still exceeds \( \sigma_n^* \) in most cases. Indeed, for all \( n \equiv 4 \pmod{8} \), we have \( \nu_n^* + n \geq \sigma_n^* \), with equality only for perfect square \( n \). For \( n \equiv 0 \pmod{8} \), we have \( \nu_n^* + n > \sigma_n^* \) for all \( n \geq 44 \). For \( n \leq 100 \) we display the exact values of \( \sigma_n^* \) and \( \nu_n^* + n \) in Table 1 below.

5. Examples

Theorem 4.2 bounds the excess of a 3-normalized Hadamard matrix from above, and by virtue of Theorem 3.1 this provides an upper bound for the determinants we can hope to achieve using the construction described at the beginning of §3. These facts would hold little interest if the construction did not actually produce examples that attain, or at least approach these upper bounds, thereby providing good lower bounds for the maximal determinant problem in the corresponding dimensions.

Our construction does produce numerous examples of this type. With regard to low orders, it generates globally determinant-maximizing sign matrices of orders \( n = 5, 13, \) and 21. By way of comparison, the maximal excess method does this for \( n = 5, 9, \) and 17, but not for \( n = 13 \) or 21. For \( n = 45, 53, \) and 69, our method reproduces the largest known determinants, reported in [OSDS]. Most significantly, we have used it to set new records for \( n = 49, 65, 73, 77, 85, 93, \) and 97.

Theorem 3.1 makes it clear that to set records of this type using our construction, we need to find 3-normalized Hadamard matrices of large excess. In particular, to improve upon the maximal excess technique, we need to satisfy condition (24).
The general literature of Hadamard matrices provides a variety of techniques for constructing Hadamard matrices, and explicit examples of relatively low order \((n < 200, \text{ say})\) abound on the internet. Unfortunately, we are unable to predict, based on construction technique or structural elements, for example, which of these matrices will have large excess after 3-normalization.

We have therefore searched for large-excess 3-normalized Hadamard matrices using an approach with two main steps. Namely,

1. Generate initial Hadamard matrices from distinct equivalence classes in \(\text{Had}(n)\), and then
2. Find a matrix in each class which attains the maximum excess subject to the 3-normalization constraint.

A program we wrote to perform the latter task runs in polynomial time and has served us well for \(n < 100\) or so. Finding initial Hadamards which can be 3-normalized with high excess, however, poses real difficulty in general. Starting in dimension 56 for the case \(n \equiv 0\), and dimension 92 for the case \(n \equiv 4 \pmod{8}\), we have not yet succeeded in finding 3-normalized Hadamard matrices with excess achieving our upper bound \(\nu_n^*\).

We next discuss our approach to the two tasks above.

**Generating initial Hadamards.** For orders \(n \equiv 4 \pmod{8}\), online libraries of Williamson and so-called “good” matrices \[Se\] provide a rich source of initial Hadamard matrices. When \(n \equiv 0 \pmod{8}\), however, one finds fewer examples online, and we have resorted to generating our own from smaller Hadamards. The tensor product of Hadamard matrices \(H_1 \in \text{Had}(s_1)\) and \(H_2 \in \text{Had}(s_2)\) always belongs to \(\text{Had}(s_1 s_2)\). More generally, one can construct Hadamard matrices of order \(s_1 s_2\) by a technique known as “weaving,” given \(s_1\) matrices in \(\text{Had}(s_2)\) and \(s_2\) matrices in \(\text{Had}(s_1)\) \[Cr\]. Craigen and Kharaghani have “woven” Hadamard matrices with very high excess \[CK\]. Unfortunately weaving does not, in general, produce 3-normalized Hadamard matrices of high excess.

On the other hand, we have used another technique, the Multiplication Theorem of Agaian-Sarukhanyan, with quite good results. This Theorem constructs a Hadamard of order \(8k_1 k_2\), given \(H_1 \in \text{Had}(4k_1)\) and \(H_2 \in \text{Had}(4k_2)\). The reader may consult \[Ag\] or \[SY\] for further details.

**Excess-maximization.** Our algorithm for maximizing excess on an equivalence class of 3-normalized Hadamard matrices relies on the fact that the excess depends only on a choice of the three rows used in the 3-normalization. We make this fact precise in Lemma 5.2 below, which requires the following definition:
**Definition 5.1.** Let $S_{n}^{\pm}$ denote the group of $n \times n$ signed permutation matrices, i.e., matrices obtained by permuting the rows of an $n \times n$ diagonal matrix of $\pm 1$s. Let $S_{3,n-3}^{\pm} \subset S_{n}^{\pm}$ denote the subgroup comprising matrices with $(3,n-3)$ block-diagonal form.

**Lemma 5.2.** Suppose $N$ is a 3-normalized Hadamard matrix of order $n > 2$. Then any 3-normalized Hadamard matrix $N'$ equivalent to $N$ can be written as

$$N' = RNC, \quad \text{where } R, C \in S_{3}^{\pm},$$

and $\text{ex}(N')$ depends only on the coset to which $R$ belongs in $S_{n}/S_{3,n-3}^{\pm}$.

*Proof.* Equation (33) simply restates the definition of “equivalent” given in Defn. 2.6. The main conclusion here is the one about excess, and for that, it suffices to show $\text{ex}(RNC) = \text{ex}(N)$ whenever both matrices are 3-normalized, and $R \in S_{3,n-3}^{\pm}$.

To do so, observe that rows 1, 2, and 3 of $N$ form a $3 \times n$ submatrix with columns

$$\begin{bmatrix} + \\ + \\ + \end{bmatrix}, \quad \begin{bmatrix} - \\ - \\ - \end{bmatrix}, \quad \begin{bmatrix} - \\ + \\ + \end{bmatrix}, \quad \text{and } \begin{bmatrix} + \\ - \\ - \end{bmatrix},$$

where $+,-$ signify $\pm 1$ respectively. These vectors occur in successive blocks of length $k := n/4$, no two are mutually opposite, and signed row permutations preserve their distinctness. It follows that the signed permutation $C$ in (33) can permute columns within any one of the four $k$-blocks, or move entire $k$-blocks, but it must maintain the contiguity of each block. Further, one sees that $C$ negates all columns or none, depending on whether $R$ negates an odd or even number, respectively, of the first three rows.

Now recall from Proposition 2.9 that for each $i = 4, 5, \ldots, n$, row $i$ of $N$ has the form $(a_{i}, b_{i}, c_{i}, d_{i})$, where $a_{i}, b_{i}, c_{i}, d_{i} \in \{\pm 1\}^{k}$ all have equal excess. The facts above now force row $i$ of $NC$ to take the form

$$(a'_{i}, b'_{i}, c'_{i}, d'_{i}),$$

where we get $\{a'_{i}, b'_{i}, c'_{i}, d'_{i}\}$ by permuting $\{a_{i}, b_{i}, c_{i}, d_{i}\}$, permuting the entries of each vector, and then, possibly, negating them all. Moreover, since $R$ belongs to the subgroup $S_{3,n-3}^{\pm}$ the last $n - 3$ rows of $R \cdot NC$ equal those $NC$, modulo permutations and sign changes of entire rows. It follows that for some permutation $\sigma$ of $\{4,5,\ldots,n\}$, we have

$$\text{ex}(a'_{i}) = \text{ex}(b'_{i}) = \text{ex}(c'_{i}) = \text{ex}(d'_{i}) = \pm \text{ex}(a_{\sigma(i)}),$$

But the excesses of rows 4 through $n$ of $RNC$ must be non-negative (Definition 2.8), so the final sign in (34) must always be “$+$”. That is, rows 4 through $n$ of $N$ and $RNC$ have exactly the same excesses, modulo permutation. These rows account for the entire excess of a 3-normalized Hadamard matrix, so we are done. $\square$
The subgroup $S^\pm_{3,n-3} \subset S^\pm_3$ is clearly isomorphic to $S^\pm_3 \times S^\pm_{n-3}$, and the order of $S^\pm_n$ is clearly $2^n n!$ for any $n$. We therefore have

\[(35) \quad \# \left( S^\pm_n / S^\pm_{3,n-3} \right) = \binom{n}{3}. \]

Indeed, the $\binom{n}{3}$ matrices we get by choosing three rows of the $n \times n$ identity matrix, then exchanging them (in any order) with rows 1, 2, and 3, each represent a different coset of $S^\pm_n / S^\pm_{3,n-3}$.

Using these facts we easily find a 3-normalized matrix of maximal excess equivalent to any initial $H \in \text{Had}(n)$. We take $\mu := \binom{n}{3}$ matrices $\{R_\alpha\}_{\alpha=1}^\mu \subset S^\pm_n$, each representing a different coset of $S^\pm_n / S^\pm_{3,n-3}$, and then form the matrices

\[(36) \quad R_1 H, R_2 H, \ldots, R_\mu H \in \text{Had}(n) \]

According to Proposition 2.9, we can 3-normalize each $R_i H$ using only a signed column permutation $C_i$, and some row-negations, which we can represent by a diagonal matrix $D_i$ of $\pm 1$s, multiplying $R_i$ on the right. Such diagonal matrices clearly belong to $S^\pm_{3,n-3}$, so we now have $\binom{n}{3}$ 3-normalized Hadamard matrices $N_i$, $i = 1, 2, \ldots, \binom{n}{3}$, with

$$N_i = R_i D_i H C_i.$$ 

Since the $R_i D_i$s represent every coset of $S^\pm_n / S^\pm_{3,n-3}$, Lemma 5.2 above guarantees that among these, the $N_i$ with largest excess actually maximizes excess among all 3-normalized Hadamard matrices equivalent to $H$.

**Remark 5.3.** Already when $n = 16$, one of the five equivalence classes in $\text{Had}(16)$ fails to contain any 3-normalized matrix that achieves the bound in Theorem 4.2.

By tabulating the row sums one gets after 3-normalizing representatives from each of the $\binom{n}{3}$ cosets described above, one associates to any $H \in \text{Had}(n)$ a statistic equivalent to the profile defined by Cooper, Milas, & Wallis in [CMW].

### A table of large determinants.

For each $n \equiv 0 \pmod{4}$, $4 \leq n \leq 100$, Table 1 below displays the results of our efforts to find 3-normalized Hadamard matrices of large excess, and the large determinants they generate via our construction. Additionally, the table compares our results to those obtained using the maximal excess technique of Farmakis & Kounias, and indicates the largest known determinant of each order. The actual matrices which attain these determinants are posted on our website [OS].

We now give a detailed explanation of Table 1.

**Notation.**
| $n + 1$ | Upper bounds | Best known |
|---------|-------------|------------|
| $n + \nu_n^*$ | $\sigma_n^*$ | $n + \nu_n$ | $\sigma_n$ | $\mu_{n+1}$ | $\beta_{n+1}$ | $\mu_{n+1}/\beta_{n+1}$ |
| 5       | 8           | 8          | 8         | 3$^*$      | 3           | 1          |
| 9       | 16          | 20         | 16        | 7$^*$      | 8.25        | 0.85       |
| 13      | 48          | 36         | 48        | 15$^*$     | 15          | 1          |
| 17      | 48          | 64         | 48        | 20$^*$     | 22.98       | 0.87       |
| 21      | 96          | 80         | 96        | 29$^*$     | 32.02       | 0.91       |
| 25      | 96          | 112        | 96        | 42$^*$     | 42          | 1          |
| 29      | 152         | 140        | 152       | 45$^2/7$   | 52.85       | 0.87       |
| 33      | 160         | 172        | 160       | 55$^{1/8}$ | 64.50       | 0.85       |
| 37      | 216         | 216        | 216       | 72         | 76.90       | 0.94       |
| 41      | 240         | 244        | 240       | 90$^*$     | 90          | 1          |
| 45      | 288         | 280        | 288       | 83         | 103.77      | 0.80       |
| 49      | 336         | 324        | 336       | 96         | 118.19      | 0.81       |
| 53      | 368         | 364        | 368       | 105        | 133.21      | 0.79       |
| 57      | 448         | 408        | 384       | 400        | 114         | 148.82     | 0.77       |
| 61      | 456         | 452        | 456       | 165$^*$    | 165         | 1          |
| 65      | 560         | 512        | 528       | 512        | 148         | 181.73     | 0.81       |
| 69      | 552         | 548        | 552       | 544        | 155         | 198.98     | 0.78       |
| 73      | 656         | 600        | 624       | 580        | 174         | 216.75     | 0.80       |
| 77      | 656         | 652        | 656       | 628        | 183         | 235.02     | 0.78       |
| 81      | 752         | 704        | 704       | 704        | 196         | 253.77     | 0.78       |
| 85      | 768         | 756        | 768       | 756        | 213         | 273        | 0.78       |
| 89      | 864         | 812        | 768       | 792        | 220         | 292.69     | 0.75       |
| 93      | 888         | 872        | 864       | 828        | 239         | 312.83     | 0.76       |
| 97      | 976         | 932        | 928       | 920        | 256         | 333.42     | 0.77       |
| 101     | 1016        | 1000       | 984       | 1000       | 275         | 354.44     | 0.78       |

Table 1. Largest known excesses of order $n \equiv 0 \pmod{4}$ and determinants of order $n + 1$. $\mu_{n+1}$ encodes the largest known determinant of order $n + 1$. Compare $\mu_{n+1}$ with the corresponding factor for our determinant ($\frac{(n+\nu_n)+(n+1)}{4}$), and that of [FK] ($\frac{n+\nu_n}{4}$).

- $\sigma_n^*$ and $\sigma_n$ respectively denote the sharpest known upper bound for the maximal excess, and the largest known excess, of a Hadamard matrix of order $n$.
- $\nu_n^*$ and $\nu_n$ respectively denote the sharpest known upper bound for the excess of, and the largest known excess for, a 3-normalized Hadamard matrix of order $n$.
- $\mu_{n+1}$ and $\beta_{n+1}$ abbreviate the largest known determinant det $M_{n+1}$, and the Barba bound $B(n+1)$ (see [14]), by dividing out large integer factors.
as follows:
\[ \mu_{n+1} := \det \frac{M_{n+1}}{2^n \cdot k^{2k-1}}, \quad \beta_{n+1} := \frac{B(n+1)}{2^n \cdot k^{2k-1}}. \]

Here \( k = n/4 \), and \( M_{n+1} \) is a sign matrix of order \( n + 1 \) having largest known determinant.

### Explanatory notes.

1. **The “Upper bounds” columns.** The tabulated values for \( \sigma_n^* \) all come from [FK] Table 2. Except for \( n = 80 \) (see Remark [13]), we computed the values for \( \nu_n^* \) using Theorem [12] and we list \( n + \nu_n^* \) instead of just \( \nu_n^* \), to facilitate the key comparison indicated by (24). In each row, boldface indicates the larger of \( n + \nu_n^* \) and \( \sigma_n^* \).

2. **The “Best known” columns.** A bold entry in either column indicates that the largest known determinant of that order is produced by applying the corresponding construction to a matrix with the associated excess \( \nu_n \) or \( \sigma_n \). When neither entry is bold, neither method constructs the current record.

All values for \( \sigma_n \) come from [FK] Table 2 except for \( \sigma_{72} = 580 \) and \( \sigma_{76} = 628 \), which were reported in [OSDS].

3. **The “\( \mu_{n+1} \)” column.** Current records which can be constructed by our method are underlined. A bold entry represents a determinant that achieves a new record, reported for the first time here. Values of \( \mu_{n+1} \) corresponding to determinants known to attain \( \text{md}(n+1) \) are marked with an asterisk.

4. For \( n \leq 20 \), either the 3-normalized or maximal excess method (or both) constructs an order \( n + 1 \) sign matrix that achieves the global determinant maximum. Equivalent matrices were all constructed by earlier investigators, however: See [Mo, Wi] for \( n+1 = 5 \), [EZ] for \( n+1 = 9 \), [Ra] for \( n+1 = 13 \), [MK] for \( n + 1 = 17 \), and [CKM] for \( n + 1 = 21 \).

5. For sizes \( n + 1 = 25, 29, 33, 37, 41 \) and \( 61 \), neither our method nor that of Farmakis & Koumas constructs the largest known determinant. In dimensions \( 25, 41, \) and \( 61 \), matrices coming from block designs (SBIBDs) attain 100% of Barba’s bound \( B(n+1) \); see [Bh, Ra] for \( n + 1 = 25 \), [BHH] for \( n + 1 = 41 \), and [B] for \( n + 1 = 61 \). The largest known determinant for \( n + 1 = 33 \) was reported in [OSDS]. For \( n + 1 = 29 \) and \( 37 \), we sketch a construction for the largest known determinants below.
6. Improved results for $n + 1 = 29, 37$

The “Upper bounds” and “Best known” columns of Table 1 show that for $n + 1 = 29$, our construction achieves a determinant larger than any the maximal excess method can produce. The value $\mu_{29} = 45^{5/7}$ there, however, corresponds to the still larger determinant reported in [OSDS] using a gradient ascent algorithm. We have since discovered that the latter matrix can be formed by applying a symmetric version of our construction. To do this, we start with a matrix $H \in \text{Had}(28)$ for which both $H$ and $H^T$ satisfy a generalized 3-normalization condition, and for which both have the optimal set of row sums prescribed by Theorem 4.2. We then apply appropriately adapted versions of steps 1–4 of our construction (§3) to $H$, transpose the result, and apply the same four steps again. This produces a matrix equivalent to the one reported in [OSDS].

Hoping to profit by applying the same idea to other orders, we have so far achieved one notable success: A matrix $A \in \{-1\}^{37 \times 37}$ with $\det A = 72 \times 9^{17} \times 2^{36}$. This determinant, reported here for the first time, attains 94% of the Barba bound, and we conjecture it to be the global maximum for its order. By way of comparison, Table 1 shows that the largest determinant that either the maximal excess method or our own can hope produce is $63 \times 9^{17} \times 2^{36}$. This value has been achieved by both methods, but it represents just 82% of Barba’s bound.

Guided by the $n + 1 = 29$ case, we start by finding a matrix $H \in \text{Had}(36)$ which can be “doubly 3-normalized” with optimal row and column sums. In this dimension, the three 3-normalizing rows and columns overlap in a somewhat more complicated way than in dimension 28. This forces further modifications of the double 4-step construction described above, but the procedure is very similar.

We are currently investigating the relationship between these two examples and possible generalizations. We will publish further details of this work in our sequel to the present work. Meanwhile, we have posted both the $n + 1 = 29$ and $n + 1 = 37$ examples on our website [OS].

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