Maximal Determinants and Saturated D-optimal Designs of Orders 19 and 37

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Abstract

A saturated D-optimal design is a $\{+1, -1\}$ square matrix of given order with maximal determinant. We search for saturated D-optimal designs of orders 19 and 37, and find that known matrices due to Smith, Cohn, Orrick and Solomon are optimal. For order 19 we find all inequivalent saturated D-optimal designs with maximal determinant, $2^{30} \times 7^2 \times 17$, and confirm that the three known designs comprise a complete set. For order 37 we prove that the maximal determinant is $2^{39} \times 3^{36}$, and find a sample of inequivalent saturated D-optimal designs. Our method is an extension of that used by Orrick to resolve the previously smallest unknown order of 15; and by Chadjipantelis, Kounias and Moyssiadis to resolve orders 17 and 21. The method is a two-step computation which first searches for candidate Gram matrices and then attempts to decompose them. Using a similar method, we also find the complete spectrum of determinant values for $\{+1, -1\}$ matrices of order 13.

1 Introduction

The Maximal Determinant problem of Hadamard [12, 22] asks for the largest possible determinant of an $n \times n$ matrix whose entries are drawn from the set $\{+1, -1\}$. We are only interested in the absolute value of the determinant, since we can always change the sign of the determinant by changing the sign of a row. The problem in its full generality has been open since first posed by

Hadamard [12], and has applications to areas such as Experimental Design and Coding Theory.

We could equally well consider $\{0,1\}$ matrices. There is a well-known mapping [25] from $\{0,1\}^{(n-1)\times(n-1)}$ matrices to $\{+1,-1\}^{n\times n}$ matrices which multiplies the determinant by $(-2)^{n-1}$, and vice versa. To avoid confusion we only consider $\{+1,-1\}$ matrices. Their determinants are always divisible by 2^{n-1}, thanks to the correspondence with $\{0,1\}$ matrices. Thus, it is convenient to let D_n denote $\max|\det(R)|$, where the maximum is over all $\{+1,-1\}^{n\times n}$ matrices R, and $d_n = D_n/2^{n-1}$.

There is an extensive literature on the Maximal Determinant problem, which splits into four cases, according to the value of $n \bmod 4$. A general upper bound of

$$D_n \le n^{n/2} \tag{1}$$

on the maximal determinant applies to all the four cases, but is not achievable unless $n = 1, 2$, or $n \equiv 0 \bmod 4$. The conjecture that this bound is always achievable when $n \equiv 0 \pmod 4$ is known as the *Hadamard Conjecture*, and has been the subject of much investigation, see for example [11, 13]. Smaller upper bounds are known for each of the other three equivalence classes modulo four.

A bound which holds for all odd orders, and which is known to be sharp for an infinite sequence of orders congruent to $1 \pmod 4$, is

$$D_n \le \sqrt{(n-1)^{n-1}(2n-1)}, \tag{2}$$

due independently to Ehlich [9] and Barba [1]. A smaller upper bound, due to Ehlich [10], applies only in the case $n \equiv 3 \pmod 4$:

$$D_n \le \sqrt{(n-3)^{n-s}(n-3+4r)^u(n+1+4r)^v\left(1 - \tfrac{ur}{n-3+4r} - \tfrac{v(r+1)}{n+1+4r}\right)}\,. \tag{3}$$

Here $s = 3$ for $n = 3$ (and the factor $(n-3)^{(n-s)}$ is interpreted as 1 in this case), $s = 5$ for $n = 7$, $s = 6$ for $11 \le n \le 59$, $s = 7$ for $n \ge 63$, $r = \lfloor n/s \rfloor$, $v = n - rs$, and $u = s - v$. The complicated form of the bound (3) as compared with (2) is indicative of the extra difficulties which often seem to arise when $n \equiv 3 \pmod 4$. The bound (3) is sharp when $n = 3$; it is not known if it is sharp for any $n > 3$.

In this work we settle the smallest hitherto unresolved case of $n = 19$. This case has remained open despite higher orders (for example, 21) being solved by similar methods, mainly because the use of (2) and its generalisation when the Gram matrix has a fixed block—see Theorem 1—is much more effective in pruning the search tree than are (3) and its generalisations. All orders congruent to 3 mod 4 and larger than 19 are currently open.

In this paper we only consider odd orders. The smallest unresolved orders which are congruent to 1 mod 4 are $n = 29, 33$ and 37. Of these, we resolve $n = 37$, and improve the upper bounds for $n = 29, 33$. For a summary, see Table 1 in §7.

Our method is structurally similar to that used for $n = 15$ by Orrick [18], and by earlier authors for $n = 17$ in [17] and $n = 21$ in [4]. There are two essential steps, Gram finding and decomposition. In the cases we consider, decomposition by hand would be tedious for $n = 19$, and infeasible for larger orders. Thus, we implement a back-tracking computer search to deal with this second step, describing such an algorithm for the first time in the literature.

Our Gram-finding algorithm is discussed in §3, and our decomposition algorithms in §4. The results for order 19 are described in §5, and for order 37 in §6. In §7 we give some new upper and lower bounds for various odd orders. For orders $n = 29$, 33, 45, 49, 53 and 57 we have not been able to determine D_n precisely, but we have reduced the gap between the known upper and lower bounds. Finally, in §8 we also find the complete spectrum of determinant values for $\{+1, -1\}$ matrices of order 13. Previously, the spectrum was only known for orders up to 11.

2 Definitions

$\mathbb{Z}$ denotes the integers, and $\mathbb{N}_1$ the positive integers. The following definitions are largely taken from [18], to which we refer for further technical definitions.

Definition 1. *A* design *is an $m \times n$ matrix with entries drawn from the set $\{+1, -1\}$. If $m = n$ the design is called* saturated*. If the absolute value of the determinant of the saturated design is maximal for its order, the design is called* D-optimal*.*

In this paper we consider saturated D-optimal designs of odd order. It is convenient to consider "normalized" designs, leading to the next definition:

Definition 2. *A vector with elements in $\{+1, -1\}$ is* parity normalized *iff it has an even number of positive elements. A design is* parity normalized *iff all its rows and columns are parity normalized.*

It is easy to show, as in [9, Lemmas 3.1, 3.2], that any saturated design of odd order can be converted to a unique parity normalized matrix by a series of negations of rows and columns.

If R_1 is a design, then any signed permutation of the rows and columns of R_1 gives another design R_2, which we can regard as equivalent to the original design since $|\det(R_1)| = |\det(R_2)|$. We can also change the signs of any rows and/or columns of without changing more than the sign of the determinant. This suggests the following definition, in which a signed permutation matrix is a permutation of the rows or columns of a diagonal matrix $\mathrm{diag}(\pm 1, \pm 1, \ldots, \pm 1)$.

Definition 3. *Two designs R and S are* Hadamard equivalent *iff $S = PRQ$ for some pair of signed permutation matrices (P, Q).*

Definition 4. *If R is a design, then $G = RR^T$ is called the* Gram matrix *of R, and $H = R^T R$ is called the* dual Gram matrix *of R.*

Definition 5. *Two symmetric matrices G_1 and G_2 are* Gram equivalent *iff $G_1 = PG_2P^T$ for some signed permutation matrix P.*

Definition 6. *Let $d_{min} > 0$ and let $\mathcal{M}_{n,p}$ be the set of square matrices M, of order p, $1 \leq p \leq n$, satisfying properties 1–3 below.*

1. *M is symmetric and positive definite;*
2. *$M_{i,i} = n$;*
3. *$M_{i,j} \equiv n \pmod 4$.*

A matrix $M \in \mathcal{M}_{n,p}$ is called a candidate principal minor. *If, furthermore, $n = p$ and the following additional properties 4–5 hold:*

4. *$\det(M) = d^2$ for $d \in \mathbb{Z}$;*
5. *$d \geq d_{min}$;*

then M is called a candidate Gram matrix.

It is clear that Properties 1, 2, 4 and 5 of candidate Gram matrices are satisfied by all Gram matrices. Furthermore, Property 3 of candidate Gram matrices holds for Gram matrices $G = RR^T$ if R is assumed to be parity normalized.

3 Gram-finding Algorithm

We summarize our Gram-finding algorithm below. The method is essentially that described in greater detail in [18]. We search for candidate Gram matrices whose determinant is greater than or equal to a positive parameter $d^2_{\min}$.

1. Set $r = 1$ and start from the candidate principal minor $M_1 = (n)$.

2. Increment r. Build a list of *admissible* vectors f, and *allowable* vectors γ (for details see [18]).

3. For each possible lexicographically maximal matrix M_{r-1} of order $r-1$, and each admissible vector f, construct the matrix

$$M_r = \begin{bmatrix} M_{r-1} & f \\ f^T & n \end{bmatrix}. \tag{4}$$

   If $r = n$,

   (a) if $\det(M_r) = d^2 \geq d^2_{\min}$, output the candidate Gram matrix M_r.

   If $r < n$,

   (b) evaluate

$$d = \begin{vmatrix} M_r & \gamma \\ \gamma^T & 1 \end{vmatrix} \tag{5}$$

   for each allowable vector γ, looking for a "good d", namely d such that the function u_r in Theorem 1 satisfies $u_r(1, d) \geq d^2_{\min}$. If a good d is found, try to extend M_r by recursively calling the algorithm (starting at step 2).

Pruning at step 3(b) of the above algorithm relies on the following Theorem, originally used by Moyssiadis and Kounias [17] to find a maximal Gram matrix of order $n = 17$. Our version below contains a sharper bound (9) applicable when $n \equiv 3 \pmod 4$.

Theorem 1. [Enhanced Kounias & Moyssiadis] *Let* $M = \begin{bmatrix} M_r & B \\ B^T & A \end{bmatrix}$ *be a symmetric, positive definite matrix of order* n *with elements taken from a set* Φ *whose members are greater than or equal in magnitude to some number* c*,* $0 < c \leq n$*. Here* M_r *is a candidate principal minor of order* $r \leq n$*, and* A *is a square matrix of order* $n - r$*, with diagonal elements* $A_{i,i} = n$*. The columns of the* $r \times (n-r)$ *matrix* B *are taken from some set* $\Gamma_r \subseteq \Phi^r$*. Define* d^* *and* γ^* *by*

$$d^* = \begin{vmatrix} M_r & \gamma^* \\ \gamma^{*T} & c \end{vmatrix} = \max_{\gamma \in \Gamma_r} \begin{vmatrix} M_r & \gamma \\ \gamma^T & c \end{vmatrix} . \tag{6}$$

Then

$$\det(M) \leq u_r(c, d^*), \tag{7}$$

where

$$u_r(c, d) = (n - c)^{n-r-1} \left[(n - c) \det(M_r) + (n - r) \max(0, d) \right] .$$

Furthermore, if $n \equiv 3 \pmod 4$*, then the following bounds apply:*

$$\begin{aligned} \det(M) \quad \leq \quad & (n-1)^{n-r} \det(M_r) + \\ & [(n-1)^{n-r} - (n-3)^{n-r} - (n-r)(n-3)^{n-r-1}] \max(0, d^*) \end{aligned} \tag{8}$$

and, assuming $\det M_r > (n-3) \det M_{r-1}$*,*

$$\det(M) \leq \max_k \max_{\substack{b_1,\ldots,b_k \in \mathbb{N}_1 \\ b_1 + \ldots + b_k = n-r}} \max_{\gamma_1^*, \ldots, \gamma_k^* \in \Gamma_r} \det \left[\begin{array}{c|ccc} M_r & \gamma_1^* j_{b_1}^T & \cdots & \gamma_k^* j_{b_k}^T \\ \hline j_{b_1} \gamma_1^{*T} & (n-3) I_{b_1} + 3 J_{b_1} & \cdots & -J_{b_1, b_k} \\ \vdots & \vdots & \ddots & \vdots \\ j_{b_k} \gamma_k^{*T} & -J_{b_k, b_1} & \cdots & (n-3) I_{b_k} + 3 J_{b_k} \end{array} \right] \tag{9}$$

where M_{r-1} *is the principal* $(r-1)$*-by-*$(r-1)$ *minor of* M_r*,* j_a *is the column vector of dimension* a *whose elements all equal 1,* $J_{a,b}$ *is the* a*-by-*b *matrix whose elements all equal 1, and* $J_a = J_{a,a}$*.*

Proof. For a proof of inequalities (7) and (8) we refer to [18, Theorem 3.1 and Corollary 3.3]. A proof of (9) is sketched in the Appendix. □

The bound (9) is sharp and therefore potentially much more powerful than (7) or (8). Unfortunately, the multidimensional search for the optimal set of block sizes $(b_1, \ldots, b_k)$, and the optimal set of vectors, $\{\gamma_j^*\}$ is expensive. We therefore restricted its use to the situation where the non-diagonal elements of the last column of M_r all equal -1. This allows us to assume that all γ_j^* consist entirely of elements -1, and we are left only with the search for the optimal partition. Much of the computation associated with the latter search need only be done once. The use of (9) resulted in an approximately 15% improvement in running time.

4 Decomposition Algorithm

The output of the program described in the previous section is a list $\mathcal{L}$ of candidate Gram matrices, complete in the sense that it contains one representative of each Gram equivalence class with determinant $\geq d_{\min}^2$ for a given bound $d_{\min}$. We need to determine if any $G \in \mathcal{L}$ decomposes as a product $G = RR^T$ for some square $\{+1, -1\}$ matrix R. This section describes several algorithms for carrying out this task.

For each candidate G this involves a (possibly large) combinatorial search. It may be regarded as searching a tree, where each level of the tree corresponds to one row of the matrix R. At level k we know $k-1$ rows of R and try to find a k-th row satisfying the constraints. Each node at the k-th level corresponds to one possible choice of the k-th row of R, given the preceding rows. If $G = RR^T$ has solutions, then the solution matrices, R, correspond to nodes at level n of the tree. In principle our procedure may generate many Hadamard-equivalent solutions. We prune the tree so as to limit the number of duplicate solutions produced.

The search algorithm relies on a family of constraints. The zeroth member of the family is a special case which can be implemented with a single Gram matrix and we call this constraint the *single-Gram constraint*. The rest of the family require both the Gram matrix $G = RR^T$ and the dual Gram matrix $H = R^T R$ and we call these *Gram-pair constraints*.

Our decomposition algorithm differs from that described in [18] in several respects. First, it builds up R by rows, instead of by rows and columns simultaneously. Second, it uses more general Gram-pair constraints (see (14) with $j \geq 2$ below).

For clarity, we first describe a version of the algorithm which uses only the single-Gram constraint.

4.1 Decomposition using only the single-Gram constraint

Denote the elements of G by $g_{i,j}$ for $i, j = 1, .., n$, and the rows of R by r_i for $i = 1, \ldots, n$. Then the constraint $RR^T = G$ is equivalent to

$$r_i r_j^T = g_{i,j} \tag{10}$$

for $1 \leq i \leq j \leq n$. The search tree is created by application of these constraints. An outline of the basic algorithm is as follows. The main work is done by a recursive procedure `search`(k) which searches an (implicit) subtree at level k, where the root is at level 1.

Algorithm using the single-Gram constraint, version 1

1. Initialize *level* $k = 1$, *first row* $r_1 = (1, 1, \ldots, 1)$ and $R = r_1$.
2. Call $\texttt{search}(k)$.
3. Output "no solution" and halt.
4. $\texttt{search}(k)$: If $k = n$, output the solution R and halt. Otherwise increment k. Find all solutions $r_k \in \{+1, -1\}^n$ of the (under-determined) set of simultaneous linear equations:

$$\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_{k-1} \end{bmatrix} r_k^T = \begin{bmatrix} g_{1,k} \\ g_{2,k} \\ \vdots \\ g_{k-1,k} \end{bmatrix}$$

   For each solution r_k, append r_k to R and call $\texttt{search}(k)$ recursively to search the relevant subtree. Return to the caller (i.e. backtrack).

We justify the choice of the first row in the above algorithm by observing that $G = RR^T$ is invariant under a signed permutation of columns of R, i.e. $R \mapsto RP$ for any signed permutation matrix P.

The above algorithm considers a large number of equivalent partial solution matrices R, and is impractical for all but very small orders. We can obtain a vastly more efficient algorithm by imposing an ordering constraint on the $+1$'s and -1's in row-vectors. We do this by defining the concept of "framings" and a new set of associated variables called "frame variables" which we use in Step 4 instead of r_k. We first define these terms, and then give an improved version of the algorithm.

At each level k, we create a partition of the indices $\{1, \ldots, n\}$ into *frames*, where a frame is a nonempty contiguous set of indices; and the collection of frames is called a *framing*. A framing of size m is defined by a *frame-widths vector* $w = (w_1, \ldots, w_m) \in \mathbb{N}_1^m$, $\sum w_i = n$, where w_i is the size of the i-th frame. At level 1 the framing consists of a single frame $\{1, \ldots, n\}$ with frame-width vector $w = (n)$. At each subsequent level, the framing is a refinement of the framing from the previous level. We use the framing at level $k - 1$ to define the frame variables that we use at level k in the following algorithm. The frame variable x_i gives the number of $+1$ entries in the k-th row of R, considering only the column indices given by the i-th frame. Thus, the number of -1 entries is $w_i - x_i$ and the sum of the entries is $2x_i - w_i$ (see equation (11)).

Algorithm using the single-Gram constraint, version 2

1. Initialize the *level* $k = 1$, the *frame-size* $m = 1$ and the *frame-width-vector* $w = (w_1) = (n)$. Set $q_1 = (+1)$ and $Q = q_1$. [In the course of the algorithm, q_i is a column vector of size $k-1$ or k, and Q is a matrix whose columns depend on the q_i. Also, w may be thought of as a vector of weights corresponding to the columns of Q.]

2. Call `search`(k).

3. Output "no solution" and halt.

4. `search`(k): If $k = n$, output the solution Q and halt [here $m = n$]. Otherwise increment k.

   Define integer variables $x_1, x_2, \ldots, x_m$. Find all solutions to the following integer programming problem:

$$Q \begin{bmatrix} 2x_1 - w_1 \\ 2x_2 - w_2 \\ \vdots \\ 2x_m - w_m \end{bmatrix} = \begin{bmatrix} g_{1,k} \\ g_{2,k} \\ \vdots \\ g_{k-1,k} \end{bmatrix} \tag{11}$$

   subject to

$$0 \le x_i \le w_i \text{ for } 1 \le i \le m. \tag{12}$$

   For each solution, update w and Q as follows:

   (a) Let $w := (x_1, w_1 - x_1,\ x_2, w_2 - x_2,\ \ldots,\ x_m, w_m - x_m)$.

   (b) Recall that $Q = (q_1, q_2, ..., q_m)$ is a matrix of column vectors q_i, each of length $k-1$. Update Q to a $k \times 2m$ matrix as follows:
   $Q := \begin{bmatrix} q_1 & q_1 & q_2 & q_2 & \cdots & q_m & q_m \\ +1 & -1 & +1 & -1 & \cdots & +1 & -1 \end{bmatrix}.$

   (c) Compress Q by removing all columns which correspond to zeros in w.

   (d) Compress w by removing all zero entries.

   (e) Set $m := \text{length}(w)$.

   Call `search`(k) recursively to search the relevant subtree. When all solutions have been processed, return to the caller (i.e. backtrack).

In procedure `search`(k) of version 2 we use Gaussian elimination with column pivoting in order to find a $(k-1) \times (k-1)$ nonsingular minor of Q (this is always possible, since the Gram matrix G is positive definite). We then solve for the corresponding $k-1$ *basic* variables in terms of the remaining $m - k + 1$ *non-basic* variables. The non-basic variables are chosen exhaustively as integers in the appropriate intervals given by (12); the basic variables are then determined uniquely (as real numbers). If the non-basic variables are not in $\mathbb{Z}$ or violate the bounds (12), the solution is discarded. It is preferable to choose as non-basic variables the variables with the smallest upper bounds w_i, provided that the resulting $(k-1) \times (k-1)$ minor is nonsingular. A heuristic for accomplishing this is to weight the columns in proportion to the bounds w_i before performing the Gaussian elimination.

We illustrate an iteration of the algorithm with an example. Consider the case $n = 7$ and the candidate Gram matrix (here and elsewhere we may abbreviate "-1" by "$-$"):

$$G = \begin{bmatrix} 7 & 3 & - & - & - & - & - \\ 3 & 7 & - & - & - & - & - \\ - & - & 7 & 3 & - & - & - \\ - & - & 3 & 7 & - & - & - \\ - & - & - & - & 7 & 3 & - \\ - & - & - & - & 3 & 7 & - \\ - & - & - & - & - & - & 7 \end{bmatrix}.$$

Suppose we are at level $k = 3$ in the search. At this stage the search tree has not branched yet, so there is just one matrix Q:

$$Q = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & - & - \\ 1 & - & 1 & - \end{bmatrix}$$

Associated with Q is the frame-widths vector (at depth 3) which is

$$w = (2, 3, 1, 1).$$

We comment that, translated into the language of the algorithm in version 1, Q and w together correspond to a 3×7 matrix R:

$$\begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & - & - \\ 1 & 1 & - & - & - & 1 & - \end{bmatrix}.$$

To find the next row of Q, we define 4 ($= m = |w|$) new variables x_1, x_2, x_3, x_4. The interpretation is that x_1 represents the number of "+1"s in the first $w_1 = 2$ entries of row 4, x_2 represents the number of "+1"s in the next $w_2 = 3$ entries of row 4, as so on. We use the constraints imposed by $g_{1,4}, g_{2,4}, g_{3,4}$, giving the linear system

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & - & - \\ 1 & - & 1 & - \end{bmatrix} \begin{bmatrix} 2x_1 - 2 \\ 2x_2 - 3 \\ 2x_3 - 1 \\ 2x_4 - 1 \end{bmatrix} = \begin{bmatrix} - \\ - \\ 3 \end{bmatrix}.$$

The two integer solutions which satisfy this system as well as the bounds $0 \le x_1 \le 2$, $0 \le x_2 \le 3$, $0 \le x_3 \le 1$, $0 \le x_4 \le 1$ given by equation (12) are $(x_1, x_2, x_3, x_4) = (1, 1, 1, 0)$ and $(2, 0, 0, 1)$. These generate two children in the search tree, with Q and w as follows:

$$Q = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & - & - \\ 1 & 1 & - & - & 1 & - \\ 1 & - & 1 & - & 1 & - \end{bmatrix} \text{ with } w = (1, 1, 1, 2, 1, 1);$$

and

$$Q = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & - & - \\ 1 & - & 1 & - \\ 1 & - & - & 1 \end{bmatrix} \text{ with } w = (2, 3, 1, 1).$$

The first Q leads to a solution; the second does not.

4.2 Decomposition using Gram-pair constraints

The algorithm (version 2) outlined in §4.1, using only the single-Gram constraint, quickly becomes infeasible due to the size of the search space. It can be improved by noting that, since the list $\mathcal{L}$ is complete, it must include a matrix H Gram-equivalent to $R^T R$. By permuting columns of R, we can assume that $H = R^T R$. This relation allows us to prune the search more efficiently than if we did not know H.

Recall that the characteristic polynomial of a square matrix A is the monic polynomial $P(\lambda) = \det(\lambda I - A)$. Since $H = R^T G (R^T)^{-1}$, the matrices G and H are similar, so they have the same characteristic polynomial.

Thus, the refined strategy is to consider each pair $(G, H) \in \mathcal{L}^2$, such that G and H have the same characteristic polynomial, and try to find R such that $G = RR^T$, $H = R^T R$. If we have considered (G, H) there is no need to consider (H, G) since this would correspond to the dual solution R^T.

More precisely, consider the constraint

$$G^{j+1} = (RR^T)^{j+1} = R(R^T R)^j R^T = RH^j R^T. \tag{13}$$

We say that the *degree* of such a constraint is $j + 1$, since the elements of G (not R) occur with degree $j + 1$. The case $j = 0$ corresponds to the single-Gram constraint considered in §4.1. For $j = 1$ we get the degree 2 constraint

$$G^2 = RHR^T$$

considered in [18]. The use of Gram-pair constraints with $j > 1$ is a new element of our algorithm. In principle, we could get different constraints for $j = 0, 1, \ldots, n - 1$. For $j \ge n$ the Cayley-Hamilton theorem implies that we get nothing new.

To apply Gram-pair constraints for pruning when only the first $k-1$ rows of R are known, partition the matrices appearing in (13) into corresponding blocks:

$$R = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}, \quad G^{j+1} = \begin{bmatrix} G_{1,1}(j+1) & G_{1,2}(j+1) \\ G_{2,1}(j+1) & G_{2,2}(j+1) \end{bmatrix}, \quad H^j = \begin{bmatrix} H_{1,1}(j) & H_{1,2}(j) \\ H_{2,1}(j) & H_{2,2}(j) \end{bmatrix}$$

say, where R_1 has $k-1$ (known) rows. Then we can use the constraints

$$G_{1,1}(j+1) = R_1 H_{1,1}(j) R_1^T \tag{14}$$

since it only involves the known rows of R. The matrices G^{j+1} and H^j need only be computed once.

Observe that $H_{1,1}(j)$ for $j \geq 2$ depends on all the entries in H. This suggests that (14) with $j \geq 2$ may be more effective for pruning than the "degree 2" case $j = 1$. In practice, we found that it was worthwhile to use (14) with both $j = 1$ and $j = 2$, but not with $j > 2$.

When using Gram-pair constraints for pruning, we can no longer assume that the first row of R is $(1, 1, \ldots, 1)$. The algorithm (version 2) of §4.1 has to be modified so step 1 starts with level $k = 0$, Q empty, and a frame-widths vector w which is compatible with H, in the sense that H is invariant under permutations of rows (and corresponding columns) within each frame. For example, if we take $H = G$ in the example of order 7 above, we can choose $w = (2, 2, 2, 1)$ as the initial frame-widths vector.

We remark that we used three variants of the decomposition algorithm outlined in this subsection. One variant attempts to find a decomposition or (by failing to do so) to prove that a decomposition of a given pair (G, H) does not exist. A second variant finds all possible decompositions, up to Hadamard equivalence. The output typically includes many solutions that are Hadamard equivalent, so we use McKay's program *nauty* [15] to remove all but one representative of each equivalence class after transforming the problem to a graph isomorphism problem [14]. A third variant is nondeterministic and attempts to traverse the search tree by choosing one or more children randomly at each node. This variant is useful in difficult cases where the deterministic variants take too long (see §6.2 for an example).

4.3 Proving indecomposability using the Hasse–Minkowski criterion

A complementary approach to the decomposition problem, or, more properly, to proofs of indecomposability, makes use of the Hasse–Minkowski theorem on rational equivalence of quadratic forms. The use of this theorem has a long history in design theory, originating with its use by Bruck and Ryser in their proof of their nonexistence result for certain finite projective planes [3]. Tamura recently applied the theorem to the question of decomposability of candidate Gram matrices with block structure [27].

Theorem 2. *Let A and B be symmetric, nonsingular rational matrices of the same dimension. Then there exists a rational matrix R such that $B = RAR^T$ if and only if*

1. $\det A/\det B$ *is a rational square, and*

2. *the p-signatures of A and B agree for all primes p and for $p = -1$.*

The criterion is implemented by finding rational matrices U and V such that UAU^T and VBV^T are diagonal—this can always be done—and then by comparing the p-signatures of the resulting matrices for all primes dividing any of the diagonal elements. The p-signature of a diagonal form is defined in [7, Chapter 15, §5.1].

The application of this theorem is as follows: there is no decomposition of the form $RR^T = G$, $R^TR = H$ if there is a $j \geq 0$ for which G^{j+1} fails to be rationally equivalent to H^j or for which H^{j+1} fails to be rationally equivalent to G^j. As was the case in the application of the Gram-pair constraint in back-tracking search, we need only check the criterion for $j < n$.

The Hasse–Minkowski criterion is sometimes a competitive alternative to the backtracking algorithm in ruling out the existence of a decomposition. On certain Gram matrix pairs for which the back-tracking search ruled out a decomposition only after exploring the search tree to great depth, the Hasse–Minkowski criterion ruled out any decomposition with a relatively fast computation. In most cases, however, back-tracking search is the much faster method, especially when rational equivalence fails only for large j, in which case the large-integer arithmetic needed to implement the Hasse–Minkowski criterion can become prohibitively expensive. Furthermore, in a small number of cases, the Hasse–Minkowski theorem fails entirely to rule out a decomposition where backtracking search succeeds. It is surprising that this occurs relatively infrequently, as the existence of a decomposition with R rational would appear to be a far milder constraint than the existence of a decomposition with R a $\{+1, -1\}$ matrix.

5 The Maximal Determinant for Order 19

For order 19, known designs due to Smith [26], Cohn [6] and Orrick and Solomon [24] are D-optimal, as we now show.

Theorem 3. *The maximal determinant of $\{+1, -1\}$ order 19 matrices is*

$$2^{30} \times 7^2 \times 17 = 833 \times 4^6 \times 2^{18}. \tag{15}$$

There are precisely three corresponding equivalence classes of saturated D-optimal designs with representatives R_1, R_2 and R_3 indicated in Figure 2. There are two corresponding (Gram equivalence classes of) Gram matrices, $G_1 = R_1R_1^T = R_1^TR_1$ and $G_2 = R_2R_2^T = R_2^TR_2 = R_3R_3^T = R_3^TR_3$ – see Figure 1.

Proof. A computational proof of Theorem 3 is described in §§5.1–5.2. □

Remark 1. *The maximal determinant given by* (15) *is smaller by a factor* $17/\sqrt{304} \approx 0.975$ *than the Ehlich bound* (3) *for* $n = 19$.

5.1 Candidate Gram-finding for order 19

In the algorithm described in §3 we used $d_{\min} = 833 \times 4^6 \times 2^{18}$ since $\{+1, -1\}$ matrices with this determinant were known to exist. Our candidate Gram-finding program took 826 hours[1] to find nine equivalence classes of candidate Gram matrices and to rule out any others.

For the nine candidate Gram matrices G, the values of $\sqrt{\det(G)}/2^{30}$ were 840 (five times), 836.0625 (once), 836 (once), and 833 (twice). The matrices are available from the website [2].

$$G_1 = \begin{bmatrix}
n & 3 & 3 & 3 & 3 & 3 & 3 & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & n & 3 & 3 & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & 3 & n & 3 & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & 3 & 3 & n & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & - & - & - & n & 3 & 3 & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & - & - & - & 3 & n & 3 & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & - & - & - & 3 & 3 & n & - & - & - & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & n & 3 & 3 & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & 3 & n & 3 & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & 3 & 3 & n & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & n & 3 & 3 & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & 3 & n & 3 & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & 3 & 3 & n & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & n & 3 & 3 & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & 3 & n & 3 & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & 3 & 3 & n & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & n & 3 & 3 \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & 3 & n & 3 \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & 3 & 3 & n
\end{bmatrix}$$

$$G_2 = \begin{bmatrix}
n & - & - & 3 & - & - & 3 & - & - & 3 & - & - & - & - & - & - & - & - & - \\
- & n & 3 & 3 & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
- & 3 & n & 3 & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & 3 & 3 & n & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - \\
- & - & - & - & n & 3 & 3 & - & - & - & - & - & - & - & - & - & - & - & - \\
- & - & - & - & 3 & n & 3 & - & - & - & - & - & - & - & - & - & - & - & - \\
3 & - & - & - & 3 & 3 & n & - & - & - & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & n & 3 & 3 & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & 3 & n & 3 & - & - & - & - & - & - & - & - & - \\
3 & - & - & - & - & - & - & 3 & 3 & n & - & - & - & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & n & 3 & 3 & - & - & - & - & - & - \\
- & - & - & - & - & - & - & - & - & - & 3 & n & 3 & - & - & - & - & - & - \\
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- & - & - & - & - & - & - & - & - & - & - & - & - & n & 3 & 3 & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & 3 & n & 3 & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & 3 & 3 & n & - & - & - \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & n & 3 & 3 \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & 3 & n & 3 \\
- & - & - & - & - & - & - & - & - & - & - & - & - & - & - & - & 3 & 3 & n
\end{bmatrix}$$

Figure 1: Optimal Gram matrices for $n = 19$. Here "$-$" stands for "-1".

[1] Computer times mentioned here and below are for a single 2.3GHz Opteron processor. In cases where the search could easily be parallelised, we sometimes used several processors running in parallel. Our candidate Gram-finding program actually took 188 hours using several processors, each operating on part of the search tree. Our programs were written in C and used the GMP package to perform multiple-precision arithmetic.

5.2 Decomposition for order 19

Our decomposition program found that seven of the candidate Gram matrices were indecomposable, but the last two decomposed (as expected). The running time was only 0.85 sec. Nevertheless, it would be extremely tedious to attempt to replicate the search by hand, since it involves visiting about 1400 nodes in the search trees.

The nine matrices have distinct characteristic polynomials, so we only had to consider the case $G = RR^T = H = R^T R$. Only the two candidate Gram matrices with smallest determinant were decomposable, and these decomposed in three ways, giving three Hadamard classes of designs (maxdet matrices) of order 19. See Figure 1 for the Gram matrices (note that they differ only in the first row and column), and Figure 2 for two of the three designs. The third design R_3 can be obtained from R_2 by a switching operation, as indicated in Figure 2.

A variant of our decomposition program exhaustively searches for all possible decompositions (up to equivalence) of a given pair (G, H). Running this program on (G_1, G_1) gave 110592 matrices in 36 seconds. Using McKay's program *nauty* [14, 15], we verified that they were all equivalent to R_1. Similarly, on (G_2, G_2) we obtained 3456 matrices in 3 seconds, and *nauty* verified that 1728 were equivalent to R_2, and the remaining 1728 were equivalent to R_3. Thus, there are precisely three inequivalent designs with maximal determinant.

6 The Maximal Determinant for Order 37

The case of order 37 was handled in much the same way as order 19. Although 37 is much larger than 19, we have $37 \equiv 1 \bmod 4$, and typically the cases $1 \bmod 4$ are easier than the cases $3 \bmod 4$ (as one can see from the summary at [22]). This is partly because Theorem 1 gives a sharper bound when $n \equiv 1 \bmod 4$.

We established that, for order 37, a known design, found previously by Orrick and Solomon [21], is D-optimal. The design is not unique, but the corresponding Gram matrix is (up to equivalence).

Theorem 4. *The maximal determinant of $\{+1, -1\}$ order 37 matrices is*

$$72 \times 9^{17} \times 2^{36} = 2^{39} \times 3^{36}. \tag{16}$$

A representative R of one equivalence class of saturated D-optimal designs is indicated in Figure 4. The corresponding Gram matrix is $G = RR^T = R^T R$ as shown in Figure 3. Moreover, G is unique, up to equivalence.

$$R_1 = \begin{bmatrix}
+ & - & - & - & - & - & - & + & + & + & + & + & + & + & + & + & + & + & + \\
- & + & - & - & - & - & - & - & - & - & - & + & + & - & + & + & - & + & + \\
- & - & + & - & - & - & - & - & - & - & + & - & + & + & - & + & + & - & + \\
- & - & - & + & - & - & - & - & - & - & + & + & - & + & + & - & + & + & - \\
- & - & - & - & + & - & - & + & + & + & + & - & - & - & + & - & - & - & + \\
- & - & - & - & - & + & - & + & + & + & - & + & - & - & - & + & + & - & - \\
- & - & - & - & - & - & + & + & + & + & - & - & + & + & - & - & - & + & - \\
+ & + & + & + & - & - & - & - & + & + & + & - & - & - & - & + & - & + & - \\
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+ & - & + & - & + & - & + & - & + & - & - & + & - & + & + & + & - & - & - \\
+ & - & - & + & + & + & - & - & - & + & - & - & + & + & + & + & - & - & - \\
+ & + & - & - & + & + & - & - & + & - & - & - & - & + & - & - & + & + & + \\
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+ & - & - & + & + & - & + & + & - & - & - & - & - & - & - & + & + & + & + \\
+ & + & - & - & + & - & + & - & - & + & + & + & + & - & - & - & + & - & - \\
+ & - & + & - & + & + & - & + & - & - & + & + & + & - & - & - & - & + & - \\
+ & - & - & + & - & + & + & - & + & - & + & + & + & - & - & - & - & - & +
\end{bmatrix}$$

$$R_2 = \begin{bmatrix}
- & + & + & - & + & + & - & + & + & - & - & - & - & - & - & - & - & - & - \\
+ & - & - & - & \oplus & \ominus & + & - & + & + & - & - & - & \oplus & \ominus & + & + & - & - \\
+ & - & - & - & \ominus & \oplus & + & + & - & + & - & - & - & \ominus & \oplus & + & - & + & - \\
- & - & - & + & + & + & + & + & + & + & - & - & - & + & + & - & - & - & + \\
+ & - & + & + & - & - & - & - & + & + & + & - & - & - & - & - & - & + & + \\
+ & + & - & + & - & - & - & + & - & + & - & + & - & - & - & - & + & - & + \\
- & + & + & + & - & - & + & + & + & + & - & - & + & - & - & - & + & + & - \\
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- & - & - & + & + & + & - & - & - & - & - & - & + & - & - & + & + & + & +
\end{bmatrix}$$

Figure 2: Two inequivalent saturated D-optimal designs of order 19. Here "−" stands for "−1" and "+" stands for "+1". A third inequivalent design R_3 is the same as R_2 except that the circled entries have their signs reversed (this is an example of "switching", see Orrick [19]).

Remark 2. *The maximal determinant given by* (16) *is smaller by a factor* $8/\sqrt{73} \approx 0.936$ *than the Ehlich-Barba bound* (2) *for* $n = 37$.

$$G = \begin{bmatrix} 37 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 5 & 1 & \dots & 1 \\ 5 & 37 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 37 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 37 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 37 & 1 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 1 & 37 & 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 1 & 1 & 37 & 1 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 1 & 1 & 1 & 37 & 1 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 37 & 1 & 1 & \dots & 1 \\ 5 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 37 & 1 & \dots & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 37 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & \dots & 37 \end{bmatrix}$$

Figure 3: The optimal Gram matrix for $n = 37$. All omitted entries are 1.

The matrix R in Figure 4 was constructed by Orrick and Solomon from a doubly 3-normalized Hadamard matrix of order 36. There are at least 78 (and probably many more) inequivalent designs, as we discuss below.

6.1 Candidate Gram matrices for order 37

Our backtracking program with bound $d_{\min} = 2^{39}3^{36}$ (93.6% of the Ehlich-Barba bound) took 77 hours to find 807 candidate Gram matrices. These had 284 distinct determinants Δ^2 in the range $\Delta/(2^{39}3^{32}) \in [81, 85]$. The candidate Gram matrices are available from the website [2].

6.2 Decomposition for order 37

We applied our decomposition program to all pairs (G, H) of candidate Gram matrices where G and H had the same characteristic polynomial. There were 489 different characteristic polynomials, and 1528 pairs (G, H) to consider. The decomposition algorithm took 257 seconds to show that 806 of the candidate Gram matrices did not decompose (in no case could more than two rows of R be constructed).

For the remaining candidate, which was in fact equivalent to the Gram matrix G shown in Figure 3, the program was stopped after running for 147 hours and exploring about 1.7×10^8 nodes (reaching level 26 of the tree).

A variant of our decomposition program uses a randomised search – at each node of the tree being searched, we choose to explore one (or sometimes two) children selected uniformly at random. Using this randomised search program we can decompose G, in fact we have now found 39 solutions. Finding one solution takes on average about 125 hours. By also considering duals, we get 78 solutions. Some (but not all) of these can be obtained from a Hadamard matrix of order 36, in the same way as the matrix R

of Figure 4. Since all 78 solutions are inequivalent, we expect that many more inequivalent solutions exist. The known solutions are available from the website [2].

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

Figure 4: A saturated D-optimal design of order 37, constructed by Orrick and Solomon. Here "−" stands for "−1" and "+" stands for "+1".

7 Improved Bounds for Various Orders

Recall that d_n is the maximal determinant for order n, divided by the known factor 2^{n-1}. Table 1 summarises the best known upper and lower bounds on d_n for orders $n = 19, 29, 33, 37, 45, 49, 53, 57$ (we omit $n = 25, 41, 61$ because for these orders the Ehlich-Barba bound (2) is attained). The figures in parentheses are the ratios of the entries to the Ehlich-Barba bound (for $n \equiv 1 \bmod 4$) or the Ehlich bound (for $n \equiv 3 \bmod 4$), rounded to three decimals.

For $n = 19$ and $n = 37$, the upper and lower bounds are equal, and thus optimal ($d_n = u = \ell$ in these cases). In the other cases the upper bounds are unattainable, so $d_n \in [\ell, u)$. In all cases the upper bounds are new, and for $n = 45$ the lower bound is new (the previous best lower bound was 83×11^{21}).

The last column gives the number of equivalence classes of candidate Gram matrices G with $\det(G) \geq (2^{n-1}u)^2$.

order n	lower bound ℓ		upper bound u		Gram count
19	833×4^6	(0.975)	833×4^6	(0.975)	9
29	320×7^{12}	(0.865)	329×7^{12}	(0.889)	9587
33	441×8^{14}	(0.855)	470×8^{14}	(0.911)	13670
37	8×9^{18}	(0.936)	8×9^{18}	(0.936)	807
45	89×11^{21}	(0.858)	99×11^{21}	(0.953)	1495
49	96×12^{23}	(0.812)	114×12^{23}	(0.965)	168
53	105×13^{25}	(0.788)	129×13^{25}	(0.968)	220
57	133×14^{27}	(0.894)	145×14^{27}	(0.974)	128

Table 1: Bounds on the (scaled) maximal determinant d_n

7.1 Discussion

Let $k = \lfloor n/4 \rfloor$. From the summary at [22] we observe that, in the cases $k \leq 3$ where d_{4k+3} is known precisely, d_{4k+3} is divisible by k^{2k-1}. However, our result for $n = 19$ shows that this pattern does not continue, for d_{19} is not divisible by 4^7.

In all cases where d_{4k+1} is known precisely ($k \leq 6$ and $k = 10, 15, 28, \ldots$), d_{4k+1} is divisible by k^{2k-1}. This is easily seen to be true if the Ehlich-Barba bound (2) is attainable (d_{4k+1} is divisible by k^{2k} in such cases), but it is also true for $k = 2, 4, 5$, where the Ehlich-Barba bound is not attainable.

For $n = 29$, we ruled out 9587 candidate Gram matrices to show that $d_{29} < 329 \times 7^{12}$. If d_{29} is divisible by 7^{13}, then we must have $d_{29} = 322 \times 7^{12} = 46 \times 7^{13}$, since this is the only multiple of 7^{13} in the allowable interval $[320 \times 7^{12}, 329 \times 7^{12})$. However, all attempts to construct an example of order 29 with $|\det|/2^{28} > 320 \times 7^{12}$, using hill-climbing or constructions based on Hadamard matrices of order 28, have failed. Thus, the plausible conjecture that d_{4k+1} is divisible by k^{2k-1} may well be false. An attempt to reduce the upper bound u to 322×7^{12} is underway but may not be feasible with our current resources – so far we have generated 16683 candidate Gram matrices (taking about two processor-years) but estimate that there are about 220000 in all.

For $n = 33$ we ruled out 13670 candidate Gram matrices to establish an upper bound of $u = 470 \times 8^{14}$. It is unlikely that we can reduce u much further without improvements in the candidate Gram-finding program, since it took about two processor-years to generate the candidates for $u = 470$, though only about six hours to show that none of them decompose.

For $n = 45$, the new lower bound of 89×11^{21} was established by a construction using a doubly 3-normalized Hadamard matrix of order 44. Details will appear elsewhere.

8 The Spectrum for Order 13

The *spectrum* S_n of the determinant function for $\{+1, -1\}$ matrices is defined to be the set of values taken by $|\det(R_n)|/2^{n-1}$ as R_n ranges over all $n \times n$ $\{+1, -1\}$ matrices. For $2 \le n \le 7$, the spectrum includes all integers between 0 and d_n. The spectrum for $n = 8$ was first computed by Metropolis, Stein, and Wells [16], who found that gaps occur, in fact $S_8 = \{0, 1, \ldots, 18, 20, 24, 32\}$. A (non-computer-based) proof of the existence of gaps was later given by Craigen [8]. At present, the spectrum is known for $n \le 11$ and (given here for the first time) for $n = 13$. The results for $n = 9$ are due to Živković [28] (and, independently, Charalambides [5]), those for $n = 10$ are due to Živković [28], and those for $n = 11$ are due to Orrick [18]. The spectra for $n \le 11$, and conjectured spectra for $n = 12$ and $14 \le n \le 17$, may be found at [23]. Here we give only the spectrum for $n = 13$, using the notation $a..b$ as a shorthand to represent the interval $\{x \in \mathbb{Z} : a \le x \le b\}$.

Theorem 5. *The spectrum for order* 13 *is*
$S_{13} = \{0..2172, 2174..2185, 2187..2196, 2199..2202, 2205, 2208, 2210, 2211, 2214..2218, 2220..2226, 2228, 2229, 2230, 2232, 2233, 2235, 2238, 2240, 2241, 2243..2245, 2247, 2248, 2250, 2253, 2256, 2258..2260, 2262, 2264, 2265, 2267, 2268, 2271, 2272, 2274, 2277, 2280, 2283, 2286, 2288, 2292, 2295, 2296, 2304, 2307, 2312, 2313, 2316, 2319, 2320, 2322, 2325, 2328, 2331, 2334, 2336, 2340, 2343, 2344, 2349, 2352, 2355, 2360, 2361, 2367, 2368, 2370, 2373, 2376, 2385, 2394, 2400, 2403, 2406, 2421, 2430, 2432, 2439, 2457, 2472, 2484, 2496, 2511, 2520, 2538, 2560, 2583, 2592, 2619, 2646, 2673, 2835, 2916, 3159, 3645\}$.

Proof. The proof is computational. Using a heuristic algorithm described in [20, pg. 34], we found examples of order 13 matrices with all 2173 determinants $0, 1 \times 2^{12}, 2 \times 2^{12}, \ldots, 2172 \times 2^{12}$. The first "gap" was at 2173×2^{12}. We ran the Gram-finding program of §3 with lower bound $d_{\min} = 2173 \times 2^{12}$. It produced 8321 candidate Gram matrices in 73 minutes. We then ran the decomposition program of §4 which found (in 48 seconds) that 1643 of the candidate Gram matrices decomposed, giving 130 distinct determinants in the range $[2174, 3645]$. These are listed in the statement of the theorem. $\square$

Appendix: Proof of new bound (9) in Theorem 1

The proof is a generalisation Ehlich's proof [9] of the bound (3) on the maximal determinant, which applies in the case $n \equiv 3 \pmod 4$. Ehlich's proof shows the following.

(1) The candidate principal minor of maximal determinant has non-diagonal elements equal to either -1 or 3.

(2) It is a *block matrix*, which means that the non-diagonal 3s occur in square blocks along the diagonal.

(3) In the case that the candidate principal minor is a candidate Gram matrix, that is, its size is n, the number of blocks is s, with u blocks of size $\lfloor n/s \rfloor$ and v blocks of size $\lfloor n/s \rfloor + 1$, where s, u, and v are defined following (3).

We generalise this to the case where the candidate principal minor contains a fixed principal submatrix M_r. If such a candidate principal minor of maximal determinant is written as

$$\begin{bmatrix} M_r & B \\ B^T & A \end{bmatrix},$$

then our result, assuming the hypothesis $\det M_r > (n-3)\det M_{r-1}$, is that A satisfies properties (1) and (2) above, and the submatrices of B corresponding to blocks of A consist of repeated columns. The generalisation of (3) depends on M_r and is not unique in general.

From now on, we take $n \equiv 3 \pmod 4$ and $n > 3$. Define

$$\begin{aligned} \mathfrak{C}_m = &\{C_m | C_m = (c_{ij}), c_{ij} = c_{ji}, C_m \text{ is pos. def.}, c_{ii} = n, \\ &c_{ij} \equiv n \pmod 4, i, j = 1 \dots m\}. \end{aligned} \tag{17}$$

and

$$\mathfrak{E}_m = \{E_m | E_m \in \mathfrak{C}_m \text{ and the leading } r \times r \text{ submatrix of } E_m \text{ is } M_r\}. \tag{18}$$

Define C_m^* and E_m^* (which may not be unique) by the conditions

$$\begin{aligned} \det C_m^* &= \max\{\det C_m | C_m \in \mathfrak{C}_m\}, \\ \det E_m^* &= \max\{\det E_m | E_m \in \mathfrak{E}_m\}. \end{aligned}$$

The first thing Ehlich proves (Theorem 2.1) is that $\det C_m^* > (n-3)\det C_{m-1}^*$ for $2 \le m \le n$. To explain the use of this theorem, we first introduce a notation. If $C_m \in \mathfrak{C}_m$ then define $\tilde{C}_m$ be the matrix that results from replacing the last diagonal element of C_m by 3, i.e. $\tilde{C}_m = (\tilde{c}_{ij})$ where

$$\tilde{c}_{ij} = \begin{cases} 3 & \text{if } i = j = m \\ c_{ij} & \text{otherwise.} \end{cases}$$

Expanding $\det C_m^*$ by minors on its last row, we find

$$\det C_m^* - \det \tilde{C}_m^* = (n-3)\det C_{m-1} \le (n-3)\det C_{m-1}^* \qquad (19)$$

where C_{m-1} is the leading $(m-1)\times(m-1)$ submatrix of C_m^*. (Note that $\tilde{C}_m^*$ is the result of applying the tilde operation to C_m^*.) The theorem then implies that $\det \tilde{C}_m^* > 0$ and therefore that $\tilde{C}_m^*$ is positive definite. This becomes important in later proofs when evaluating determinants that arise as the result of column operations.

For the generalization to our case, we appear to need the extra condition $\det \tilde{M}_r > 0$. This cannot be expected to hold in general. Consider for example,

$$M_2 = \begin{bmatrix} 11 & 7 \\ 7 & 11 \end{bmatrix} \qquad (20)$$

for which $\det \tilde{M}_2 < 0$. For now, we leave it as a question for empirical study whether the condition holds often enough in practical searches for the following considerations to be useful.

Theorem 6. *Let $1 \le r \le m$, let $M_r \in \mathfrak{C}_r$, and let $\det \tilde{M}_r > 0$. Then the set of elements $E_m \in \mathfrak{C}_m$ for which $\det \tilde{E}_m > 0$ is non-empty.*

Proof. We prove the theorem by induction on m. For the base case, $m = r$, the matrix $M_r \in \mathfrak{C}_r$ satisfies $\det \tilde{M}_r > 0$ by assumption. Now assume that the theorem holds for all $\mathfrak{C}_k$ with $r \le k \le m$. We want to show that it holds for $\mathfrak{C}_{m+1}$. Let E_m be an element of $\mathfrak{C}_m$ for which $\det \tilde{E}_m > 0$, and write this element as

$$E_m = \begin{bmatrix} C_{m-1} & \gamma \\ \gamma^T & n \end{bmatrix}. \qquad (21)$$

Form the matrix

$$E_{m+1} = \begin{bmatrix} C_{m-1} & \gamma & \gamma \\ \gamma^T & n & 3 \\ \gamma^T & 3 & n \end{bmatrix}. \qquad (22)$$

Subtracting column m from column $m+1$ and expanding by minors on column $m+1$ we find that $\det E_{m+1} = (n-3)\det E_m + (n-3)\det \tilde{E}_m$. Both terms are positive, which means that $\det E_{m+1}$ is positive, and therefore that E_{m+1} is positive definite and hence an element of $\mathfrak{C}_{m+1}$. By a similar computation $\det \tilde{E}_{m+1} = (n-3)\det \tilde{E}_m > 0$. Therefore E_{m+1} is a suitable element. □

Theorem 7. *Let $1 \le r < m$, let $M_r \in \mathfrak{C}_r$, and let $\det \tilde{M}_r > 0$. Then*

$$\det E_m^* > (n-3)\det E_{m-1}^*.$$

Proof. When $m = r + 1$ we write

$$M_r = \begin{bmatrix} C_{r-1} & \gamma \\ \gamma^T & n \end{bmatrix} \tag{23}$$

and define

$$E_{r+1} = \begin{bmatrix} C_{r-1} & \gamma & \gamma \\ \gamma^T & n & 3 \\ \gamma^T & 3 & n \end{bmatrix}. \tag{24}$$

From the proof of the previous theorem we know that $E_{r+1} \in \mathfrak{E}_{r+1}$ and $\det \tilde{E}_{r+1} > 0$. Now $\det E^*_{r+1} \geq \det E_{r+1} = (n-3)\det M_r + (n-3)\det \tilde{M}_r > (n-3)\det M_r = (n-3)\det E^*_r$.

We now proceed by induction. Assume that $\det E^*_m > (n-3)\det E^*_{m-1}$. Write

$$E^*_m = \begin{bmatrix} E_{m-1} & \gamma \\ \gamma^T & n \end{bmatrix} \tag{25}$$

and define

$$E_{m+1} = \begin{bmatrix} E_{m-1} & \gamma & \gamma \\ \gamma^T & n & 3 \\ \gamma^T & 3 & n \end{bmatrix}. \tag{26}$$

Now $\det E_{m+1} = (n-3)\det E^*_m + (n-3)\det \tilde{E}^*_m$. Note that $\det E^*_m = (n-3)\det E_{m-1} + \det \tilde{E}^*_m \leq (n-3)\det E^*_{m-1} + \det \tilde{E}^*_m$. From the induction hypothesis, it follows that $\det \tilde{E}^*_m > 0$, and so $\det E_{m+1} > (n-3)\det E^*_m$. □

This proof contains the proof of an important corollary:

Corollary 8. *Let $1 \leq r \leq m$, let $M_r \in \mathfrak{C}_r$, and let $\det \tilde{M}_r > 0$. Then $\det \tilde{E}^*_m > 0$.*

We now generalize Ehlich's Theorem 2.2. Again we need the assumption that $\det \tilde{M}_r > 0$.

Theorem 9. *Let $1 \leq r \leq m$, let $M_r \in \mathfrak{C}_r$, and let $\det \tilde{M}_r > 0$. Write*

$$E^*_m = \begin{bmatrix} M_r & B \\ B^T & A \end{bmatrix},$$

where $A = (a_{ij})$ and $B = (b_{ij})$ satisfy the conditions in the definition of $\mathfrak{E}_m$. Then for $i \neq j$ we have $a_{ij} = -1$ or 3.

Proof. When $m = r$ or $r + 1$ the statement is vacuously true. So we assume $m \geq r + 2$. Suppose there is an element $a_{ij} = c \neq -1$ or 3 for $i \neq j$. Then $|c| > 3$. We may assume that the element is positioned so that $i = m - 1$, $j = m$, so that we may write

$$E^*_m = \begin{bmatrix} E_{m-2} & \alpha & \beta \\ \alpha^T & n & c \\ \beta^T & c & n \end{bmatrix}.$$

By interchanging the last two rows and last two columns, if necessary, we may assume that

$$\det \begin{bmatrix} E_{m-2} & \alpha \\ \alpha^T & n \end{bmatrix} \leq \det \begin{bmatrix} E_{m-2} & \beta \\ \beta^T & n \end{bmatrix}.$$

We now claim that the matrix

$$E_m = \begin{bmatrix} E_{m-2} & \beta & \beta \\ \beta^T & n & 3 \\ \beta^T & 3 & n \end{bmatrix}$$

has larger determinant than E_m^*, a contradiction. To establish the claim, evaluate both determinants:

$$\det E_m^* = (n-3) \det \begin{bmatrix} E_{m-2} & \alpha \\ \alpha^T & n \end{bmatrix} + \det \tilde{E}_m^*$$
$$\det E_m = (n-3) \det \begin{bmatrix} E_{m-2} & \beta \\ \beta^T & n \end{bmatrix} + \det \tilde{E}_m$$

By Corollary 8, $\tilde{E}_m^*$ is positive definite. Symmetric row and column operations do not affect positive definiteness, so we get

$$\det \tilde{E}_m^* = \det \begin{bmatrix} E_{m-2} & \alpha & \beta \\ \alpha^T & n & c \\ \beta^T & c & 3 \end{bmatrix} = \det \begin{bmatrix} E_{m-2} & \beta & \alpha - \frac{c}{3}\beta \\ \beta^T & 3 & 0 \\ \alpha^T - \frac{c}{3}\beta^T & 0 & n - \frac{c^2}{3} \end{bmatrix}$$
$$\leq \left(n - \frac{c^2}{3}\right) \det \begin{bmatrix} E_{m-2} & \beta \\ \beta^T & 3 \end{bmatrix}.$$

We evaluate $\det \tilde{E}_m$ by subtracting column m from column $m-1$ and doing expansion by minors on column $m-1$ to obtain

$$\det \tilde{E}_m = (n-3) \det \begin{bmatrix} E_{m-2} & \beta \\ \beta^T & 3 \end{bmatrix}.$$

Since $|c| > 3$ we have $\det \tilde{E}_m^* < \det \tilde{E}_m$ and therefore $\det E_m^* < \det E_m$. $\square$

Now we want to generalize Ehlich's Theorem 2.3. First a useful lemma about block matrices. (See Ehlich's paper for the formal definition of block.)

Lemma 10. *A symmetric matrix $A = (a_{ij})$ with diagonal elements n is a block matrix if and only if its non-diagonal elements are all -1 or 3 and for any $i \neq j$ such that $a_{ij} = 3$ the columns i and j differ only in their i^{th} and j^{th} elements.*

Proof. If A is a block matrix, the statement is clearly true. For the converse, let (i,j) be the position of one of the 3s of A. Define $i_1 = j$, $i_2 = i$, and let $\{i_2, i_3, \ldots, i_p\}$ be the set of all indices h for which $a_{hj} = 3$. Let $2 \le k \le p$. Then $a_{i_k j} = 3$ means that the i_k^{th} element of column j is 3. Let $1 \le \ell \le p$, $\ell \ne k$. Then since columns i_ℓ and j agree in their i_k^{th} element we have $a_{i_k i_\ell} = 3$ for all $k \ne \ell$.

For an index $h \notin \{i_1, \ldots, i_p\}$ we have $a_{hj} = -1$. But since columns j and i_ℓ, $1 \le \ell \le p$, agree in their h^{th} element, we have $a_{hi_\ell} = -1$ for all $1 \le \ell \le p$. Therefore the set of indices $\{i_1, \ldots, i_p\}$ forms a block. Hence every one of the 3s in A lies in a block, and A is a block matrix. $\square$

Now for the generalization of Ehlich's Theorem 2.3.

Theorem 11. *Let $1 \le r \le m$, let $M_r \in \mathfrak{C}_r$, and let $\det \tilde{M}_r > 0$. Write*

$$E_m^* = \begin{bmatrix} M_r & B \\ B^T & A \end{bmatrix},$$

where $A = (a_{ij})$ and $B = (b_{ij})$ satisfy the conditions in the definition of $\mathfrak{E}_m$. If for some $i \ne j$, $a_{ij} = 3$, then columns i and j of B are equal and columns i and j of A are equal except for their i^{th} and j^{th} elements.

Proof. By Theorem 9 we know that the non-diagonal elements of A are -1 or 3. As before, the theorem is vacuously true if $m = r$ or $m = r + 1$. Assume $m \ge r + 2$ and let A have an element 3, say in position $(m-1, m)$. Write

$$E_m^* = \begin{bmatrix} M_r & B_1 & \beta_{m-1} & \beta_m \\ B_1^T & A_1 & \alpha_{m-1} & \alpha_m \\ \beta_{m-1}^T & \alpha_{m-1}^T & n & 3 \\ \beta_m^T & \alpha_m^T & 3 & n \end{bmatrix}.$$

We assume, as we may (by swapping the last two rows and last two columns if necessary), that

$$\det \begin{bmatrix} M_r & B_1 & \beta_{m-1} \\ B_1^T & A_1 & \alpha_{m-1} \\ \beta_{m-1}^T & \alpha_{m-1}^T & n \end{bmatrix} \le \det \begin{bmatrix} M_r & B_1 & \beta_m \\ B_1^T & A_1 & \alpha_m \\ \beta_m^T & \alpha_m^T & n \end{bmatrix}.$$

Our goal is now to show that $\beta_{m-1} = \beta_m$ and $\alpha_{m-1} = \alpha_m$. Suppose that this is not the case. We claim that $\det E_m > \det E_m^*$ where

$$E_m = \begin{bmatrix} M_r & B_1 & \beta_m & \beta_m \\ B_1^T & A_1 & \alpha_m & \alpha_m \\ \beta_m^T & \alpha_m^T & n & 3 \\ \beta_m^T & \alpha_m^T & 3 & n \end{bmatrix}.$$

Write

$$\det E_m^* = (n-3) \det \begin{bmatrix} M_r & B_1 & \beta_{m-1} \\ B_1^T & A_1 & \alpha_{m-1} \\ \beta_{m-1}^T & \alpha_{m-1}^T & n \end{bmatrix} + \det \tilde{E}_m^*$$

and

$$\det E_m = (n-3)\det \begin{bmatrix} M_r & B_1 & \beta_m \\ B_1^T & A_1 & \alpha_m \\ \beta_m^T & \alpha_m^T & n \end{bmatrix} + \det \tilde{E}_m.$$

The first term on the right in $\det E_m^*$ is no larger than the first term on the right in $\det E_m$, and we will see that the second term of $\det E_m^*$ is strictly smaller than the second term of $\det E_m$. By subtracting row and column m of $\tilde{E}_m$ from row and column $m-1$ of $\tilde{E}_m$ and expanding by minors on column $m-1$ we find that

$$\det \tilde{E}_m = (n-3)\det \begin{bmatrix} M_r & B_1 & \beta_m \\ B_1^T & A_1 & \alpha_m \\ \beta_m^T & \alpha_m^T & 3 \end{bmatrix}.$$

On the other hand, using Corollary 8, which implies that $\tilde{E}_m^*$ is positive definite, and evaluating the determinant as we did for $\det \tilde{E}_m$, we find that

$$\det \tilde{E}_m^* < (n-3)\det \begin{bmatrix} M_r & B_1 & \beta_m \\ B_1^T & A_1 & \alpha_m \\ \beta_m^T & \alpha_m^T & 3 \end{bmatrix}.$$

This follows because $\alpha_{m-1} - \alpha_m$ and $\beta_{m-1} - \beta_m$, which together form the first $m-2$ elements of column $m-1$ in the expansion by minors, are not both zero. □

Corollary 12. *The matrix A in Theorem 11 is a block matrix.*

Proof. We have proved in Theorems 9 and 11 that both of the conditions needed in Lemma 10 for A to be a block matrix hold. □

Our conclusion is that, when $\det \tilde{M}_r > 0$, the maximal determinant completion E_m^* of M_r takes a form where A is a block matrix with some number k of blocks whose sizes we will denote $b_1, b_2, \ldots, b_k$, and where $B = \begin{bmatrix} B_1 & \ldots & B_k \end{bmatrix}$ with each of the matrices B_j a rank-1 matrix consisting of a column β_j^* repeated b_j times. This establishes (9).

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