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D-optimal weighing designs for $n \equiv -1 \pmod 4$ objects and a large number of weighings

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Abstract

Let $M_{m,n}(0,1)$ denote the set of all $m \times n$ (0, 1)-matrices and let

$$G(m,n) = \max\left\{\det X^{\mathrm{T}}X : X \in M_{m,n}(0,1)\right\}.$$

In this paper we exhibit some new formulas for $G(m,n)$ where $n \equiv -1 \pmod 4$. Specifically, for $m = nt + r$ where $0 \leqslant r < n$, we show that for all sufficiently large t, $G(nt+r,n)$ is a polynomial in t of degree n that depends on the characteristic polynomial of the adjacency matrix of a certain regular graph. Thus the problem of finding $G(nt+r,n)$ for large t is equivalent to finding a regular graph, whose degree of regularity and number of vertices depend only on n and r, with a certain "trace-minimal" property. In particular we determine the appropriate trace-minimal graph and hence the formulas for $G(nt+r,n)$ for $n = 11, 15$, all r, and all sufficiently large t.

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1. Introduction

Let $M_{m,n}(0,1)$ denote the set of all $m \times n$ (0, 1)-matrices and let

$$G(m,n) = \max\left\{\det X^{\mathrm{T}}X : X \in M_{m,n}(0,1)\right\}.$$

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A matrix $X = (x_{ij}) \in M_{m,n}(0, 1)$ is *D-optimal* (in $M_{m,n}(0, 1)$) if $\det X^{\mathrm{T}}X = G(m, n)$.

The central problem is to find $G(m, n)$ for each pair of positive integers $m \geqslant n$ and to characterize the matrices for which the maximum is attained. In its full generality, the problem is unsolved.

This problem comes from the theory of statistical weighing designs. Suppose we have a one-pan or spring scale with which to determine the weights of n objects in m weighings. The scale does not give the exact weight, but we assume that the error distribution has mean zero and is independent from weighing to weighing. One possible design is to weigh the objects one at a time. But by choosing a more complicated weighing design in which several objects are placed on the scale together, the variance of the resulting errors can be reduced. This technique appeared in a paper by Yates [16] in 1935 and was improved and advanced by Hotelling [7] and Mood [10] in 1944 and 1946.

A *weighing design* for n objects and m weighings consists of m subsets of the n objects. Each subset of objects is then placed on the scale together. Letting the objects correspond to the columns and the weighings correspond to the rows, we can encode the weighing design into a matrix $X \in M_{m,n}(0, 1)$: $x_{ij} = 1$, if object j is included in the ith weighing; $x_{ij} = 0$, if it is omitted. Thus a matrix $X \in M_{m,n}(0, 1)$ is called a *design matrix*. Under certain assumptions about the error distribution of the scale, the smallest confidence region for the least-squares estimator of the n-tuple of weights of the n objects is attained when one uses a weighing design (matrix) for which $\det X^{\mathrm{T}}X$ is maximal; thus the interest in D-optimal design matrices (see e.g. [15,2] for details).

Formulas for $G(m, n)$ are known for $n = 2, 3, 4, 5, 6$ and all $m \geqslant n$. For $n = 7$, $G(m, 7)$ is known for all sufficiently large m. See [8] for $n = 2, 3$, [12,13] for $n = 4, 5, 6$, and [14] for $n = 7$. For some other values of n, partial results are known—partial in the sense that $G(m, n)$ is known for some, but not all, m. Complete results for $n = 3$ and 7 are given in the next two theorems. The first theorem was stated in [10, p. 443] and proved in [8, p. 562].

Theorem 1. *For* $0 \leqslant r < 3$

$$G(3t + r, 3) = 4(t + 1)^r t^{3-r}.$$

The next theorem was conjectured in [8] and proved in [14].

Theorem 2. *For* $0 \leqslant r < 7$ *and all sufficiently large* t

$$G(7t + r, 7) = 4 \times 2^8 (t + 1)^r t^{7-r}.$$

It is tempting to conjecture that the pattern exhibited in the cases for $n = 3, 7$ might hold for $n = 11, 15, \ldots$ as well, especially since families of $(nt + r) \times n$ design matrices X are given in [8, Theorem 7.1] for which

$$\det(X^{\mathrm{T}}X) = 4\left(\frac{n+1}{4}\right)^{n+1}(t+1)^r t^{n-r} \tag{1}$$

for all $n \equiv -1 \pmod 4$ and all $0 \leqslant r < n$. In addition, it is known that $G(nt+r,n)$ equals the right-hand side of Eq. (1) when $r = 0, 1, 2$ and $n-1$ (see for example [11, Theorem 5.2]). But for other values of r, the examples in [8] prove only that the right-hand side of Eq. (1) is a lower bound on $G(nt+r,n)$.

On the other hand, upper bounds on $G(m,n)$ for all m and n are given in [4,9] using the idea of an approximate design. In particular, for $n \equiv -1 \pmod 4$ the upper bounds on $G(nt+r,n)$ combined with the examples given in [8] give the following range of possible values for $G(nt+r,n)$:

$$4\left(\frac{n+1}{4}\right)^{n+1}(t+1)^r t^{n-r} \leqslant G(nt+r,n) \leqslant 4\left(\frac{n+1}{4}\right)^{n+1}\left(t+\frac{r}{n}\right)^n. \tag{2}$$

However the upper bound is attainable only when $r = 0$; that is, when $m = nt + r$ is a multiple of n. For $n \geqslant 11$, $G(nt+r,n)$ is not equal to the lower bound given in Eq. (1) in general. In fact for $r \neq 0, 1, 2, n-1$, the actual value of $G(nt+r,n)$ for all sufficiently large t, is strictly between the upper and lower bounds given in inequality (2).

Formulas for $n = 11, 15$, all $0 \leqslant r < n$, and large t are given in the next two theorems.

Theorem 3. *For all sufficiently large t*

$$\begin{aligned}
G(11t+0,11) &= 12(3t)^{11},\\
G(11t+1,11) &= 12(3t)^{10}(3t+3),\\
G(11t+2,11) &= 12(3t)^{9}(3t+3)^2,\\
G(11t+3,11) &= 12(3t-1)(3t)^{5}(3t+2)^5,\\
G(11t+4,11) &= 12(3t)^{5}(3t+2)^6,\\
G(11t+5,11) &= 12(3t)^{4}(3t+2)^6(3t+3),\\
G(11t+6,11) &= 12(3t)(3t+1)^{6}(3t+3)^4,\\
G(11t+7,11) &= 12(3t+1)^{6}(3t+3)^5,\\
G(11t+8,11) &= 12(3t+1)^{5}(3t+3)^5(3t+4),\\
G(11t+9,11) &= 12(3t+1)^{4}(3t+3)^5(3t+4)^2,\\
G(11t+10,11) &= 12(3t)(3t+3)^{10}.
\end{aligned}$$

Theorem 4. *For all sufficiently large t*

$$\begin{aligned}
G(15t+0,15) &= 16(4t)^{15},\\
G(15t+1,15) &= 16(4t)^{14}(4t+4),
\end{aligned}$$

$$
\begin{aligned}
G(15t+2,15) &= 16(4t)^{13}(4t+4)^2,\\
G(15t+3,15) &= 16(4t-2)(4t)^7(4t+2)^7,\\
G(15t+4,15) &= 16(4t)^7(4t+2)^8,\\
G(15t+5,15) &= 16(4t)^6(4t+2)^8(4t+4),\\
G(15t+6,15) &= 16(4t)(4t+1)^4(4t+4)^2[(4t)^2+3(4t)+1]^4,\\
G(15t+7,15) &= 16(4t)(4t+1)^8(4t+2)^2(4t+4)^4,\\
G(15t+8,15) &= 16(4t+2)^2(4t+4)[(4t)^2+4(4t)+2]^2\\
&\quad\times[(4t)^4+8(4t)^3+20(4t)^2+16(4t)+2]^2,\\
G(15t+9,15) &= 16(4t+2)^4(4t+4)^3[(4t)^2+4(4t)+2]^4,\\
G(15t+10,15) &= 16(4t)(4t+2)^8(4t+4)^6,\\
G(15t+11,15) &= 16(4t+2)^8(4t+4)^7,\\
G(15t+12,15) &= 16(4t+2)^7(4t+4)^7(4t+6),\\
G(15t+13,15) &= 16(4t+2)^4(4t+4)^3[(4t)^2+8(4t)+14]^4,\\
G(15t+14,15) &= 16(4t)(4t+4)^{14}.
\end{aligned}
$$

There is more. Our main result is that for each pair of positive integers, n, r with $n \equiv -1 \pmod 4$ and $0 \leqslant r < n$, there is a polynomial $p_{n,r}(t)$ of degree n in t such that $G(nt+r, n) = p_{n,r}(t)$ for all sufficiently large t. And we describe a relationship between this polynomial and a certain regular graph whose degree of regularity and number of vertices depend only on n and r. Once the graph G is known, the polynomial can be obtained easily from the characteristic polynomial of the adjacency matrix of G. Theorems 1–4 then follow as simple consequences.

2. Main results

The main results of this paper describe a correspondence between the formula $G(m, n)$ for D-optimal design matrices and certain regular graphs.

2.1. Trace-minimal regular graphs

We begin with a description of the relevant graphs. Let $\mathscr{G}(v, \delta)$ be the set of all δ-regular graphs on v vertices and let $A(G)$ be the adjacency matrix of G. The characteristic polynomial of $A(G)$ is denoted by $\mathrm{ch}_G(x)$. We also refer to $\mathrm{ch}_G(x)$ as the characteristic polynomial of the graph G. Since $A(G)$ is a symmetric $(0, 1)$-matrix with zeros on the diagonal, $\mathrm{tr}(A(G)) = 0$ and $\mathrm{tr}(A(G)^2) = \delta v$. These traces do not depend on the structure of the graph G. However, for $i \geqslant 3$, $\mathrm{tr}(A(G)^i)$ does depend on the structure of the graph. Indeed the (j, j) entry of $A(G)^i$ equals the number of closed walks of length i that start and end at vertex j.

We now define an order relation on the graphs in $\mathscr{G}(v,\delta)$: Let $G, H \in \mathscr{G}(v,\delta)$, We say G is *trace-dominated* by H if $A(G)$ and $A(H)$ have the same spectrum (in which case $\operatorname{tr}(A(G)^i) = \operatorname{tr}(A(H)^i)$ for all $3 \leqslant i \leqslant n$) or if there exists a positive integer $3 \leqslant k \leqslant n$ such that $\operatorname{tr}(A(G)^i) = \operatorname{tr}(A(H)^i)$, for $i < k$ and $\operatorname{tr}(A(G)^k) < \operatorname{tr}(A(H)^k)$. If G is trace-dominated by all graphs in $\mathscr{G}(v,\delta)$, then we say that G is *trace-minimal* in $\mathscr{G}(v,\delta)$. Since $\mathscr{G}(v,\delta)$ is finite, there always exist trace-minimal graphs in $\mathscr{G}(\delta, v)$ and clearly they all have the same characteristic polynomial. The equivalent graphical definition of trace-dominance is this: G is trace-dominated by H if either G and H have the same number of closed walks of length i for all $3 \leqslant i \leqslant n$ or if the number of closed walks of length i in G equals the number of closed walks of length i in H for all $i < k$ and the number of closed walks of length k in G is smaller than the number of closed walks of length k in H.

The trace-dominance relation actually compares the spectra of the (adjacency matrices of the) graphs in $\mathscr{G}(v,\delta)$ rather than the graphs themselves. In fact trace-dominance is a linear order on the spectra of graphs; G and H have the same spectrum if and only if each is trace-dominated by the other. But in general, the spectrum of a graph does not determine the graph. That is, there exist non-isomorphic graphs with the same spectrum (see [6, p. 24]). So although trace-dominance is a linear order on the spectra of graphs, there may exist non-isomorphic, trace-minimal graphs in $\mathscr{G}(v,\delta)$. We have not investigated this. We denote the spectrum of a square matrix X by $\operatorname{spec}(X)$ so that the spectrum of a graph G is denoted by $\operatorname{spec}(A(G))$.

Now we turn to the design matrices in $M_{m,n}(0,1)$. Throughout, we assume that $n = 4p - 1$ and that $m = nt + r$ where the remainder r satisfies $0 \leqslant r < n$. The main result is split into four cases depending on the congruence class of $r \pmod 4$.

2.2. *Main results for* $r \equiv 1, 2 \pmod 4$

Theorem 5. *Let $r = 4d + 1$. Let G be a trace-minimal graph in $\mathscr{G}(2p, d)$. Then for all sufficiently large values of t*

$$G(nt + r, n) = \frac{4(t+1)[\operatorname{ch}_G(pt + d)]^2}{t^2}. \tag{3}$$

Theorem 6. *Let $r = 4d + 2$. Let G be a trace-minimal graph in $\mathscr{G}(2p, p + d)$. Then for all sufficiently large values of t*

$$G(nt + r, n) = \frac{4t[\operatorname{ch}_G(pt + d)]^2}{(t-1)^2}.$$

2.3. *Bipartite-trace-minimal regular graphs*

To state the results for $r \equiv -1, 0 \pmod 4$, we need to define a notion analogous to trace-minimality for bipartite graphs. Let $\mathscr{B}(2v, \delta)$ be the set of all δ-regular bipartite graphs on $2v$ vertices and let $B \in \mathscr{B}(2v, \delta)$. It follows from the regularity of B that each of the sets of vertices in the bipartition has cardinality v. (We assume this even if $\delta = 0$.) Without loss of generality, we may assume that the sets of vertices in the bipartition are $\{1, 2, \ldots, v\}$ and $\{v + 1, v + 2, \ldots, 2v\}$. Thus the adjacency matrix of B is of the form

$$A(B) = \begin{bmatrix} 0 & N(B) \\ N(B)^{\mathrm{T}} & 0 \end{bmatrix},$$

where $N(B)$ is a $v \times v(0, 1)$-matrix having exactly δ ones in each row and each column.

It is clear that $\mathrm{tr}(A(B)^i) = 0$ if i is odd and that $\mathrm{tr}(A(B)^{2j}) = 2\mathrm{tr}((N(B)^{\mathrm{T}}N(B))^j)$ otherwise. For $j = 1$, $\mathrm{tr}(N(B)^{\mathrm{T}}N(B)) = \delta v$ for all $B \in \mathscr{B}(2v, \delta)$.

A graph $B \in \mathscr{B}(2v, \delta)$ is *bipartite-trace-minimal* in $\mathscr{B}(2v, \delta)$ if for every $H \in \mathscr{B}(2v, \delta)$ either $\mathrm{spec}(A(B)) = \mathrm{spec}(A(H))$ (in which case $\mathrm{tr}(A(B)^i) = \mathrm{tr}(A(H)^i)$ for all $i = 4, \ldots, 2v$) or there exists a positive integer k with $4 \leqslant k \leqslant 4p$ such that $\mathrm{tr}(A(B)^i) = \mathrm{tr}(A(H)^i)$ for all $i < k$ and $\mathrm{tr}(A(B)^k) < \mathrm{tr}(A(H)^k)$. In view of the remarks above, $B \in \mathscr{B}(2v, \delta)$ is bipartite-trace-minimal if and only if for every $H \in \mathscr{B}(2v, \delta)$, either $\mathrm{spec}(N(H)^{\mathrm{T}}N(H)) = \mathrm{spec}(N(B)^{\mathrm{T}}N(B))$ or there exists an integer $2 \leqslant j \leqslant v$ such that $\mathrm{tr}((N(H)^{\mathrm{T}}N(H))^i) = \mathrm{tr}((N(B)^{\mathrm{T}}N(B))^i)$ for $i < j$ and $\mathrm{tr}((N(B)^{\mathrm{T}}N(B))^j) < \mathrm{tr}((N(H)^{\mathrm{T}}N(H))^j)$.

There is a subtle difference between trace-minimality and bipartite-trace-minimality for bipartite graphs. If $B \in \mathscr{B}(4p, \delta) \subseteq \mathscr{G}(4p, \delta)$, B may be bipartite-trace-minimal in $\mathscr{B}(4p, \delta)$ without being trace-minimal in $\mathscr{G}(4p, \delta)$. Bipartite-trace-minimality requires a comparison of the traces of $A(B)^i$ with $A(G)^i$ for all $G \in \mathscr{B}(4p, \delta)$, whereas trace-minimality requires the same comparison but for all G in the larger set $\mathscr{G}(4p, \delta)$. Thus for bipartite graphs, trace-minimality is a stronger condition than bipartite-trace-minimality.

2.4. Main results for $r \equiv -1, 0 \pmod 4$

The following two theorems, which contain the main results for $r \equiv -1, 0 \pmod 4$, require the notion of bipartite-trace-minimality. Each theorem is divided into two parts depending on the relative sizes of p and d.

Theorem 7. *Let $r = 4d - 1$. Suppose $p/2 \leqslant d < p$. Let G be a trace-minimal graph in $\mathscr{G}(4p, 3p + d - 1)$. Then for all sufficiently large values of t*

$$G(nt + r, n) = \frac{4\mathrm{ch}_G(pt + d - 1)}{t - 3}. \tag{4}$$

Suppose $0 \leqslant d < p/2$. Let B be a bipartite-trace-minimal graph in $\mathscr{B}(4p, d)$. Then for all sufficiently large values of t

$$G(nt + r, n) = \frac{4(p(t - 1) + 2d)\mathrm{ch}_B(pt + d)}{t(pt + 2d)}. \tag{5}$$

Theorem 8. *Let* $r = 4d$. *Suppose* $0 \leqslant d \leqslant p/2$. *Let* G *be a trace-minimal graph in* $\mathscr{G}(4p, d)$. *Then for all sufficiently large values of* t

$$G(nt + r, n) = \frac{4\mathrm{ch}_G(pt + d)}{t}.$$

Suppose $p/2 < d < p$. *Let* B *be a bipartite-trace-minimal graph in* $\mathscr{B}(4p, p + d)$. *Then for all sufficiently large values of* t

$$G(nt + r, n) = \frac{4(pt + 2d)\mathrm{ch}_B(pt + d)}{(t - 1)(p(t + 1) + 2d)}.$$

3. Families of trace-minimal and bipartite-trace-minimal graphs

Equipped with the four theorems in Section 2, one can translate the problem of finding an explicit expression of $G(nt + r, n)$ for a given n, remainder $0 \leqslant r < n$, and all sufficiently large t into the problem of finding an appropriate trace-minimal or bipartite-trace-minimal graph. For example suppose $n = 11$ and $r = 9$ so that $p = 3$ and $r = 4d + 1$, where $d = 2$. This case falls within the scope of Theorem 5. Thus we seek a graph in $\mathscr{G}(6, 2)$ that is trace-minimal. It is not hard to see that the 6-cycle is the only trace-minimal graph in $\mathscr{G}(6, 2)$. Indeed the v-cycle graph is the only trace-minimal graph in $\mathscr{G}(v, 2)$ (see Lemma 9). The characteristic polynomial of the 6-cycle graph is $\mathrm{ch}(x) = (x + 1)^2(x - 1)^2(x + 2)(x - 2)$, $pt + d = 3t + 2$, and hence by Theorem 5 we have

$$G(11t + 9, 11) = 12(3t + 1)^4(3t + 3)^5(3t + 4)^2,$$

for all sufficiently large t.

By exhibiting appropriate families of trace-minimal and bipartite-trace-minimal graphs, we reprove the old formulas given in Theorems 1 and 2 and prove the new ones given in Theorems 3 and 4.

The notation for graphs is as follows:

Z_v	the graph consisting of v independent vertices (no edges)
K_v	the complete graph on v vertices
$K_{v,v}$	the complete bipartite graph with v vertices in each of the bipartition sets
C_v	the cycle with v vertices
$K_{2v} - vK_2$	the complete graph on $2v$ vertices with a perfect matching removed
$K_{v,v} - vK_2$	the complete bipartite graph with a perfect matching removed
$G + H$	the direct sum of graphs G and H
kG	the direct sum of k copies of G.

Even though the families of graphs in this section are relatively simple, they are sufficiently inclusive to prove all of the formulas in Theorems 1–4. A much more extensive list of trace-minimal and bipartite-trace-minimal graphs along with the corresponding formulas for $G(m, n)$ are given in a sequel [1].

Lemma 9. *The following graphs are trace-minimal*:

$$\begin{aligned}&Z_v \in \mathscr{G}(v, 0),\\&K_v \in \mathscr{G}(v, v-1),\\&vK_2 \in \mathscr{G}(2v, 1),\\&K_{v,v} \in \mathscr{G}(2v, v),\\&K_{2v} - vK_2 \in \mathscr{G}(2v, 2v-2),\\&C_v \in \mathscr{G}(v, 2).\end{aligned}$$

The following graphs are bipartite-trace-minimal:

$$\begin{aligned}&Z_v \in \mathscr{B}(v, 0),\\&vK_2 \in \mathscr{B}(2v, 1),\\&K_{v,v} - vK_2 \in \mathscr{B}(2v, v-1).\end{aligned}$$

Proof. Since Z_v is the only graph in $\mathscr{G}(v, 0)$ it must be trace-minimal and bipartite-trace-minimal in $\mathscr{B}(v, 0)$. Likewise K_v is the only graph in $\mathscr{G}(v, v-1)$, vK_2 is the only graph in $\mathscr{G}(2v, 1)$, and $K_{2v} - vK_2$ is the only graph in $\mathscr{G}(2v, 2v-1)$ so they are trace-minimal and vK_2 is bipartite-trace-minimal in $\mathscr{B}(2v, 1)$. The bipartite graph $K_{v,v} - vK_2$ is the only graph in $\mathscr{B}(2v, v-2)$, so it is bipartite-trace-minimal.

Next consider the complete bipartite graph $K_{v,v}$. It is the only graph in $\mathscr{B}(2v, v)$ so it is bipartite-trace-minimal. But $K_{v,v}$ is also trace-minimal in $\mathscr{G}(2v, v)$. To see this let $G \in \mathscr{G}(2v, v)$. If G has a 3-cycle, then $\mathrm{tr}(A(G)^3) > 0$ whereas $\mathrm{tr}(A(K_{v,v})^3) = 0$. Thus G is not trace-minimal. So suppose G has no 3-cycles and assume that vertex 1 is adjacent to vertices $v+1, \ldots, 2v$. Since G has no 3-cycles, none of the vertices $v+1, \ldots, 2v$ are adjacent to each other. Thus each of the vertices $v+1, \ldots, 2v$ is adjacent to each of the vertices $1, 2, \ldots, v$. That is, $G = K_{v,v}$.

Finally, consider the v-cycle, C_v and let $G \in \mathscr{G}(v, 2)$. Since G is 2-regular, it is a direct sum of cycles. Suppose G has a cycle of length $k < v$ and let k the minimal length of a cycle in G. Then $\mathrm{tr}(A(G)^i) = \mathrm{tr}(A(C_v)^i)$ for all $i < k$, but $\mathrm{tr}(A(G)^k) > \mathrm{tr}(A(C_v)^k)$ since G has a k-cycle and C_v does not. Hence G is not trace-minimal. It follows that the only trace-minimal graph in $\mathscr{G}(v, 2)$ is C_v. □

3.1. Proof of Theorems 1–3

In each case the trace-minimal or bipartite-trace-minimal graph required is among those listed in Lemma 9. Thus the formulas for $G(nt + r, n)$ are obtained from the corresponding theorem from Section 2. In the table below, the values of r, d, the graph class, the appropriate trace-minimal or bipartite-trace-minimal graph G in the class, and the characteristic polynomial $\mathrm{ch}_G(x)$ are given.

For example, if $n = 11$ and $r = 8$ then $p = 3$, $d = 2$ and $p/2 < d$, so we use the second part of Theorem 8. Thus we seek a bipartite-trace-minimal graph B in $\mathscr{B}(4p, p + d) = \mathscr{B}(12, 5)$. By Lemma 9, the graph $K_{6,6} - 6K_2 \in \mathscr{B}(12, 5)$ is bipartite-trace-minimal. It is easy to verify that the characteristic polynomial of $K_{6,6} - 6K_2$ is $\mathrm{ch}(x) = (x - 5)(x - 1)^5(x + 1)^5(x + 5)$ and that

$$\frac{4(3t + 4)\,\mathrm{ch}(3t + 2)}{(t - 1)(3(t + 1) + 4)} = 12(3t + 1)^5(3t + 3)^5(3t + 4).$$

Thus the formula for $G(11t + 8, 11)$ in Theorem 3 is proved. All other parts of Theorems 1–3 are proved in a similar manner.

3.1.1. $n = 3$

r	d	class	graph G	$\mathrm{ch}_G(x)$
0	0	$\mathscr{G}(4, 0)$	Z_4	x^4
1	0	$\mathscr{G}(2, 0)$	Z_2	x^2
2	0	$\mathscr{G}(2, 1)$	K_2	$(x - 1)(x + 1)$

3.1.2. $n = 7$

r	d	class	graph G	$\mathrm{ch}_G(x)$
0	0	$\mathscr{G}(8, 0)$	Z_8	x^8
1	0	$\mathscr{G}(4, 0)$	Z_4	x^4
2	0	$\mathscr{G}(4, 2)$	C_4	$(x - 2)x^2(x + 2)$
3	1	$\mathscr{G}(8, 6)$	$K_8 - 4K_2$	$(x - 6)x^4(x + 2)^3$
4	1	$\mathscr{G}(8, 1)$	$4K_2$	$(x - 1)^4(x + 1)^4$
5	1	$\mathscr{G}(4, 1)$	$2K_2$	$(x - 1)^2(x + 1)^2$
6	1	$\mathscr{G}(4, 3)$	K_4	$(x - 3)(x + 1)^3$

3.1.3. $n = 11$

r	d	class	graph G	$\mathrm{ch}_G(x)$
0	0	$\mathscr{G}(12, 0)$	Z_{12}	x^{12}
1	0	$\mathscr{G}(6, 0)$	Z_6	x^6
2	0	$\mathscr{G}(6, 3)$	$K_{3,3}$	$(x - 3)x^4(x + 3)$
3	1	$\mathscr{B}(12, 1)$	$6K_2$	$(x - 1)^6(x + 1)^6$
4	1	$\mathscr{G}(12, 1)$	$6K_2$	$(x - 1)^6(x + 1)^6$
5	1	$\mathscr{G}(6, 1)$	$3K_2$	$(x - 1)^3(x + 1)^3$
6	1	$\mathscr{G}(6, 4)$	$K_6 - 3K_2$	$(x - 4)x^3(x + 2)^2$
7	2	$\mathscr{G}(12, 10)$	$K_{12} - 6K_2$	$(x - 10)x^6(x + 2)^5$
8	2	$\mathscr{B}(12, 5)$	$K_{6,6} - 6K_2$	$(x - 5)(x - 1)^5(x + 1)^5(x + 5)$
9	2	$\mathscr{G}(6, 2)$	C_6	$(x - 2)(x - 1)^2(x + 1)^2(x + 2)$
10	2	$\mathscr{G}(6, 5)$	K_6	$(x - 5)(x + 1)^5$

3.2. Proof of Theorem 4, $n = 15$

r	d	class	graph G	$ch_G(x)$
0	0	$\mathscr{G}(16, 0)$	Z_{16}	x^{16}
1	0	$\mathscr{G}(8, 0)$	Z_8	x^8
2	0	$\mathscr{G}(8, 4)$	$K_{4,4}$	$(x-4)x^6(x+4)$
3	1	$\mathscr{B}(16, 1)$	$8K_2$	$(x-1)^8(x+1)^8$
4	1	$\mathscr{G}(16, 1)$	$8K_2$	$(x-1)^8(x+1)^8$
5	1	$\mathscr{G}(8, 1)$	$4K_2$	$(x-1)^4(x+1)^4$
6	1	$\mathscr{G}(8, 5)$	$K_8 - (C_3 + C_5)$	$(x-5)x^2(x+3)(x^2+x-1)^2$
7	2	$\mathscr{G}(16, 13)$	$K_{16} - (4C_3 + C_4)$	$(x-13)(x-1)x^8$ $\times (x+1)^2(x+3)^4$
8	2	$\mathscr{G}(16, 2)$	C_{16}	$(x-2)x^2(x+2)(x^2-2)^2$ $\times (x^4-4x^2+2)^2$
9	2	$\mathscr{G}(8, 2)$	C_8	$(x-2)x^2(x+2)(x^2-2)^2$
10	2	$\mathscr{G}(8, 6)$	$K_8 - 4K_2$	$(x-6)x^4(x+2)^3$
11	3	$\mathscr{G}(16, 14)$	$K_{16} - 8K_2$	$(x-14)x^8(x+2)^7$
12	3	$\mathscr{B}(16, 7)$	$K_{8,8} - 8K_2$	$(x-7)(x-1)^7(x+1)^7(x+7)$
13	3	$\mathscr{G}(8, 3)$	$C_8(1, 4)$	$(x-3)(x-1)^2(x+1)$ $\times (x^2+2x-1)^2$
14	3	$\mathscr{G}(8, 7)$	K_8	$(x-7)(x+1)^7$

For $r \neq 6, 7, 13$, the associated graph is among those shown to be trace-minimal or bipartite-trace-minimal in Lemma 9. Let $C_8(1, 4) \in \mathscr{G}(8, 3)$ be the graph with eight vertices and an edge (i, j) if $|i - j| \equiv 1, 4 \pmod 8$. It remains only to show that the graphs $K_8 - (C_3 + C_5)$ for $r = 6$, $K_{16} - (4C_3 + C_4)$ for $r = 7$, and $C_8(1, 4)$ for $r = 13$ are trace-minimal.

3.2.1. $K_8 - (C_3 + C_5)$

There are only three graphs G in $\mathscr{G}(8, 3)$: $K_8 - C_8$, $K_8 - 2C_4$, and $K_8 - (C_3 + C_5)$. For the first two, the value of $\mathrm{tr}(A(G)^3)$ is 96, and for the last one is 90. So $K_8 - (C_3 + C_5)$ is trace-minimal.

3.2.2. $K_{16} - (4C_3 + C_4)$

Let G be a graph in $\mathscr{G}(16, 13)$. Then the complement G' is in $\mathscr{G}(16, 2)$ and hence is a direct sum of disjoint cycles. Let $A(G') = J_{16} - I_{16} - A(G)$ be the adjacency matrix of G'. Since $A(G')J = JA(G') = 2J$, $J^2 = 16J$, and $\mathrm{tr}(A(G')^2) = 32$, we have

$$\begin{aligned}\mathrm{tr}(A(G)^3) &= \mathrm{tr}((J - I - A(G'))^3)\\ &= \mathrm{tr}(139J - (I + A(G')^3))\\ &= 139 \times 16 - \mathrm{tr}(I + 3A(G') + 3A(G')^2 + A(G')^3)\end{aligned}$$

$$= 2224 - 16 - 3(32) - \mathrm{tr}(A(G')^3)$$
$$= 2112 - \mathrm{tr}(A(G')^3).$$

Thus to minimize $\mathrm{tr}(A(G)^3)$ for $G \in \mathscr{G}(16, 13)$ it is enough to maximize $\mathrm{tr}(A(G')^3)$, i.e., the number of triangles, in the complement $G' \in \mathscr{G}(16, 2)$. But G' is a direct sum of disjoint cycles, thus it can have at most four triangles, which occurs only if $G' = 4C_3 + C_4$.

3.2.3. $C_8(1, 4)$

It is easy to see that $\mathrm{tr}(A(G)^3) = 0$ if and only if G is triangle-free. There are only two triangle-free graphs in $\mathscr{G}(8, 3)$: The graph Q obtained from the edges of a cube and $C_8(1, 4)$. Since $\mathrm{tr}(A(Q)^4) = 168$ and $\mathrm{tr}(A(C_8(1, 4))^4) = 152$, $C_8(1, 4)$ is trace-minimal.

4. Proofs of Theorems 5–8

In this section we prove Theorems 5–8. Several of the lemmas used in the section require lengthy proofs, which will be given in later sections.

4.1. A correspondence with (± 1)*-matrices*

We begin with a definition. A design matrix $X \in M_{m,n}(0, 1)$ is *balanced* if each row of X contains exactly $2p$ ones and $2p - 1$ zeros. Let $\mathrm{Bal}(m, n, (0, 1))$ denote the subset of $M_{m,n}(0, 1)$ consisting of all balanced design matrices. For all sufficiently large m, all D-optimal design matrices are balanced.

Lemma 10 [11]. *Let $n = 4p - 1$ be a positive integer. For all sufficiently large values of m, every D-optimal matrix $X \in M_{m,n}(0, 1)$ is balanced.*

We now define a map L on $\mathrm{Bal}(m, n, (0, 1))$. Let $X \in \mathrm{Bal}(m, n, (0, 1))$ where $m = nt + r$, with $0 \leqslant r < n$. Define a matrix $L(X)$ as follows:

$$L(X) = \begin{bmatrix} J_{m,1} & J_{m,n} - 2X \\ J_{t,1} & J_{t,n} \end{bmatrix}.$$

($J_{a,b}$ is the $a \times b$ matrix all of whose entries are one.) Clearly $L(X)$ is a $(4pt + r) \times 4p$, (± 1)-matrix each of whose first $(4p - 1)t + r$ rows contains exactly $2p$ ones and $2p$ negative ones and whose last t rows consist entirely of ones. We denote the set of all such matrices by $\mathscr{C}(4pt + r, 4p, \pm 1)$. It is clear that the map $L : \mathrm{Bal}(m, n, (0, 1)) \to \mathscr{C}(4pt + r, 4p, \pm 1)$ is one-to-one and onto. Furthermore, the determinants of $X^{\mathrm{T}}X$ and $L(X)^{\mathrm{T}}L(X)$ are related in the following way.

Lemma 11 [11]. *Let* $n = 4p - 1$ *be a positive integer and suppose that* $X \in \mathrm{Bal}(m, n, (0, 1))$. *Then*

$$\det L(X)^{\mathrm{T}} L(X) = t4^n \det X^{\mathrm{T}} X.$$

Thus it is clear that if $X_0 \in \mathrm{Bal}(m, n, (0, 1))$ and $Y_0 = L(X_0) \in \mathscr{C}(4pt + r, 4p, \pm 1)$ then

$$\det(Y^{\mathrm{T}} Y) \leqslant \det(Y_0^{\mathrm{T}} Y_0)$$

for all $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$ if and only if

$$\det(X^{\mathrm{T}} X) \leqslant \det(X_0^{\mathrm{T}} X_0)$$

for all $X \in \mathrm{Bal}(m, n, (0, 1))$. In view of Lemmas 10 and 11 we now focus our attention on $\mathscr{C}(4pt + r, 4p, \pm 1)$ and characterize those matrices $Y_0 \in \mathscr{C}(4pt + r, 4p, \pm 1)$ for which $\det Y^{\mathrm{T}} Y \leqslant \det Y_0^{\mathrm{T}} Y_0$ for all $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$. Such a matrix Y_0 is also called *D-optimal*.

4.2. Remainder matrices

Let S be a symmetric $4p \times 4p$ integral matrix. Then S is a *remainder matrix* if there exist $t \geqslant 0$, $0 \leqslant r < n$, and a matrix $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$ such that

$$Y^{\mathrm{T}} Y = 4pt I_{4p} + S. \tag{6}$$

In this section we give necessary and sufficient conditions for a symmetric integral matrix to be a remainder matrix and we characterize the remainder matrices S for which the corresponding design matrix Y is D-optimal for all sufficiently large t.

One property of a remainder matrix S satisfying Eq. (6) is that its diagonal entries must be r. This is clear since the diagonal entries of $Y^{\mathrm{T}} Y$ are $4pt + r$. Another, not so obvious, property is that a remainder matrix S is permutation similar to an integral block-matrix of the form

$$\begin{bmatrix} U & V \\ V^{\mathrm{T}} & W \end{bmatrix}, \tag{7}$$

where U is a $u \times u$ symmetric matrix, W is a $w \times w$ symmetric matrix, u and w are even integers with $u + w = 4p$, and there exists an integer r such that $U, W \equiv r \pmod 4$ and $V \equiv r + 2 \pmod 4$. (If either u or w is zero, then there is only one block.) A matrix in block-form (7) satisfying the above properties is said to be *blocked*. Remainder matrices are characterized in the following lemma.

Lemma 12. *Let* $S = (s_{ij})$ *be a symmetric* $4p \times 4p$ *integral matrix. Then* S *is a remainder matrix if and only if the following conditions are satisfied*:

(a) *each row of* S *sums to zero*,
(b) *there exists an integer* r *with* $0 \leqslant r < 4p - 1$ *such that* $s_{ii} = r$ *for all* i,
(c) S *is permutation similar to a blocked matrix.*

Another way to state the result in Lemma 12 is this: Let $S = (s_{ij})$ be a symmetric $4p \times 4p$ integral matrix and let $t \geqslant 0$ be an integer. Define a subset $\mathscr{Y}(S, t)$ of $\mathscr{C}(4pt + r, 4p, \pm 1)$ as follows:

$$\mathscr{Y}(S, t) = \left\{Y \in \mathscr{C}(4pt + r, 4p, \pm 1) : Y^{\mathrm{T}}Y = 4ptI_{4p} + S\right\}.$$

Lemma 12 is equivalent to the statement that there exists an integer $t_0 \geqslant 0$ for which $\mathscr{Y}(S, t_0)$ is non-empty if and only if S satisfies conditions (a)–(c). But it turns out that if S is a remainder matrix, then $\mathscr{Y}(S, t)$ is non-empty for all sufficiently large t.

Lemma 13. *Let S be a remainder matrix. Then there exists an integer t_0 such that $\mathscr{Y}(S, t)$ is non-empty for all $t \geqslant t_0$.*

Now suppose that $\mathscr{Y}(S, t)$ is non-empty. Since $Y^{\mathrm{T}}Y = 4ptI_{4p} + S$ for all $Y \in \mathscr{Y}(S, t)$, either all matrices in $\mathscr{Y}(S, t)$ are D-optimal or none are D-optimal. We say that a non-empty class $\mathscr{Y}(S, t)$ is a *D-optimal class*, if every $Y \in \mathscr{Y}(S, t)$ is a D-optimal matrix and $\mathscr{Y}(S, t)$ is a *non-D-optimal class* if none are D-optimal.

Define a subset of $\mathrm{Bal}(m, n, (0, 1))$ as follows:

$$\mathscr{X}(S, t) = \left\{X \in \mathrm{Bal}(m, n, (0, 1)) : L(X) \in \mathscr{Y}(S, t)\right\}.$$

And for $0 \leqslant r < n$, let $\mathscr{M}(r)$ stand for the set of remainder matrices whose diagonal entries equal r. It follows from Lemma 10 and the argument above that if $S \in \mathscr{M}(r)$ then $\mathscr{X}(S, t)$ is non-empty for all sufficiently large values of t. And from Lemma 11 it follows that if $X \in \mathscr{X}(S, t)$ then

$$\begin{aligned} \det X^{\mathrm{T}}X &= \frac{1}{t4^n} \det L(X)^{\mathrm{T}}L(X) \\ &= \frac{1}{t4^n} \det(4ptI_{4p} + S). \end{aligned}$$

Thus $\det X^{\mathrm{T}}X$ is the same for all $X \in \mathscr{X}(S, t)$ and it follows that either all design matrices in $\mathscr{X}(S, t)$ are D-optimal or none are D-optimal. As before, we say that $\mathscr{X}(S, t)$ is a *D-optimal class* if every $X \in \mathscr{X}(S, t)$ is a D-optimal design matrix and $\mathscr{X}(S, t)$ is a *non-D-optimal class* if none are D-optimal. We summarize the above discussion in the following lemma.

Lemma 14. *Let $S \in \mathscr{M}(r)$. For all sufficiently large t, $\mathscr{X}(S, t)$ and $\mathscr{Y}(S, t)$ are non-empty and $\mathscr{X}(S, t)$ is a D-optimal class if and only if $\mathscr{Y}(S, t)$ is a D-optimal class.*

For a given remainder matrix $S \in \mathscr{M}(r)$, it turns out that either $\mathscr{Y}(S, t)$ is a D-optimal class for all sufficiently large t or a non-D-optimal class for all sufficiently large t. In other words, there cannot be infinitely many values of t for which $\mathscr{Y}(S, t)$ is a D-optimal class and infinitely many values of t for which $\mathscr{Y}(S, t)$ is a non-D-optimal class.

4.3. Spectrum-maximal remainder matrices

We now characterize those remainder matrices S for which $\mathscr{Y}(S,t)$ is a D-optimal class for all sufficiently large t. To do so, define an order relation $\preceq$ on $\mathscr{M}(r)$ as follows: if $S_1, S_2 \in \mathscr{M}(r)$ then $S_1 \preceq S_2$ if either $\operatorname{spec}(S_1) = \operatorname{spec}(S_2)$ or there exists an integer $2 \leqslant k < 4p$ such that $E_i(S_1) = E_i(S_2)$ for $i < k$ and $E_k(S_1) < E_k(S_2)$. ($E_i(X)$ stands for the elementary symmetric functions of the eigenvalues of X. Since $E_1(S) = \operatorname{tr} S = 4pr$ for all $S \in \mathscr{M}(r)$, k must be at least 2.) A matrix $S_0 \in \mathscr{M}(r)$ is *spectrum-maximal* if $S \preceq S_0$ for every $S \in \mathscr{M}(r)$.

Theorem 15. *Let $S \in \mathscr{M}(r)$. If S is spectrum-maximal, then $\mathscr{Y}(S,t)$ and $\mathscr{X}(S,t)$ are non-empty D-optimal classes for all sufficiently large t.*

If S is not spectrum-maximal, then $\mathscr{Y}(S,t)$ and $\mathscr{X}(S,t)$ are non-empty non-D-optimal classes for all sufficiently large t.

Since $\mathscr{M}(r)$ is infinite, it is not immediately clear that each $\mathscr{M}(r)$ contains a spectrum-maximal matrix. In fact it does, as we shall see in Lemmas 16–19.

4.4. Trace-minimal graphs

To complete the proofs of Theorems 5–8 we show that every spectrum-maximal remainder matrix is associated with a trace-minimal or a bipartite-trace-minimal graph. In fact we completely characterize spectrum-maximal remainder matrices (and hence the D-optimal classes $\mathscr{X}(S,t)$) in terms of these graphs.

Rather than having to state throughout the rest of the paper that a remainder matrix is permutation similar to a blocked matrix, we will now *assume that all remainder matrices are blocked*. This assumption is harmless: if P is a $4p \times 4p$ permutation matrix and $Y \in \mathscr{C}(4pt+r, 4p, \pm 1)$ with $Y^{\mathrm{T}}Y = 4pI_{4p} + S$, then $Y_1 = YP \in \mathscr{C}(4pt+r, 4p, \pm 1)$, $Y_1^{\mathrm{T}}Y_1 = 4pI_{4p} + P^{\mathrm{T}}SP$, and $\det Y^{\mathrm{T}}Y = \det Y_1^{\mathrm{T}}Y_1$. In particular, every remainder matrix is permutation similar to a blocked remainder matrix. So now $\mathscr{M}(r)$ stands for the set of all blocked remainder matrices whose main diagonal entries equal r.

4.4.1. $r \equiv 1 \pmod 4$

Let $r = 4d+1$. Let G_1, G_2 be graphs in $\mathscr{G}(2p, d)$ and define a symmetric integral $4p \times 4p$ matrix as follows:

$$S_1(G_1, G_2) := 4dI_{4p} + \begin{bmatrix} J_{2p} - 4A(G_1) & -J_{2p} \\ -J_{2p} & J_{2p} - 4A(G_2) \end{bmatrix}. \tag{8}$$

It is easy to verify that $S_1(G_1, G_2)$ satisfies conditions (a)–(c) of Lemma 12. Thus $S_1(G_1, G_2) \in \mathscr{M}(r)$.

Lemma 16. *Let $r = 4d + 1$ and suppose that $S \in \mathscr{M}(r)$. Then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exist trace-minimal graphs G_1, G_2 in $\mathscr{G}(2p, d)$ such that $S = S_1(G_1, G_2)$.*

Furthermore, the following equation holds for all graphs G_1, G_2 in $\mathscr{G}(2p, d)$:

$$\det(4ptI_{4p} + S_1(G_1, G_2)) = \frac{4^{4p}(t+1)\mathrm{ch}_{G_1}(pt+d)\mathrm{ch}_{G_2}(pt+d)}{t}. \tag{9}$$

We should point out that since the set of graphs $\mathscr{G}(2p, d)$ is finite, there always exists a graph in $\mathscr{G}(2p, d)$ that is trace-minimal. Thus Lemma 16 guarantees the existence of a spectrum-maximal remainder matrix in $\mathscr{M}(r)$. Also notice that the assumption S is blocked allows us to state that S *equals* $S_1(G_1, G_2)$ rather than S is permutation similar to $S_1(G_1, G_2)$.

With the help of Lemma 16, we can now prove Theorem 5.

Proof of Theorem 5. Let G be a trace-minimal graph in $\mathscr{G}(2p, d)$. By Lemma 16, $S = S_1(G, G)$ is a spectrum-maximal remainder matrix in $\mathscr{M}(r)$. By Theorem 15 there exists t_0 such that the class of design matrices $\mathscr{X}(S, t)$ is non-empty, balanced, and D-optimal for all $t \geqslant t_0$. Let $X \in \mathscr{X}(S, t)$ and let $Y = L(X)$. Then by Lemma 11

$$\begin{aligned} G(nt + r, n) &= \det X^{\mathrm{T}}X \\ &= \frac{1}{t4^n}\det Y^{\mathrm{T}}Y \\ &= \frac{1}{t4^n}\det(4ptI_{4p} + S). \end{aligned}$$

Eq. (3) now follows from Eq. (9). □

4.4.2. $r \equiv 2 \pmod 4$

Let $r = 4d + 2$. Let G_1, G_2 be graphs in $\mathscr{G}(2p, p + d)$ and define a symmetric $4p \times 4p$ integral matrix as follows:

$$S_2(G_1, G_2) := 4dI_{4p} + \begin{bmatrix} 2J_{2p} - 4A(G_1) & 0 \\ 0 & 2J_{2p} - 4A(G_2) \end{bmatrix}. \tag{10}$$

As in the case $r \equiv 1 \pmod 4$ it is easy to verify that $S_2(G_1, G_2) \in \mathscr{M}(r)$.

Lemma 17. *Let $r = 4d + 2$ and suppose that $S \in \mathscr{M}(r)$. Then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exist trace-minimal graphs G_1, G_2 in $\mathscr{G}(2p, p + d)$ such that $S = S_2(G_1, G_2)$.*

Furthermore, the following equation holds for all graphs G_1, G_2 in $\mathscr{G}(2p, p + d)$:

$$\det(4ptI_{4p} + S_2(G_1, G_2)) = \frac{4^{4p}t^2\mathrm{ch}_{G_1}(pt+d)\mathrm{ch}_{G_2}(pt+d)}{(t-1)^2}. \tag{11}$$

Using Lemma 17, the Proof of Theorem 6 is almost identical to the Proof of Theorem 5 given above.

4.4.3. $r \equiv -1 \pmod 4$

Let $r = 4d - 1$. The form of a spectrum-maximal remainder matrix depends on whether $0 \leqslant d < p/2$, $p/2 < d < p$, or $d = p/2$. We define two types of matrices in $\mathscr{M}(r)$. Let G be a graph in $\mathscr{G}(4p, 3p + d - 1)$ and define

$$S_{31}(G) := 4(d-1)I_{4p} + 3J_{4p} - 4A(G). \tag{12}$$

The second remainder matrix comes from a bipartite graph B in $\mathscr{B}(4p, d)$:

$$S_{32}(B) := 4dI_{4p} + \begin{bmatrix} -J_{2p} & J_{2p} \\ J_{2p} & -J_{2p} \end{bmatrix} - 4A(B). \tag{13}$$

Lemma 18. *Let $r = 4d - 1$ and let $S \in \mathscr{M}(r)$. If $p/2 < d < p$, then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exists a trace-minimal graph G in $\mathscr{G}(4p, 3p + d - 1)$ such that $S = S_{31}(G)$.*

Furthermore, the following equation holds for all graphs G in $\mathscr{G}(4p, 3p + d - 1)$:

$$\det(4ptI_{4p} + S_{31}(G)) = \frac{4^{4p}t\,\mathrm{ch}_G(pt + d - 1)}{t - 3}. \tag{14}$$

If $0 \leqslant d < p/2$, then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exists a bipartite-trace-minimal graph B in $\mathscr{B}(4p, d)$ such that $S = S_{32}(B)$.

Furthermore, the following equation holds for all bipartite graphs B in $\mathscr{B}(4p, d)$:

$$\det(4ptI_{4p} + S_{32}(B)) = \frac{4^{4p}(p(t-1) + 2d)\mathrm{ch}_B(pt + d)}{pt + 2d}. \tag{15}$$

If $d = p/2$, then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if either there exists a trace-minimal graph G in $\mathscr{G}(4p, 7p/2 - 1)$ such that $S = S_{31}(G)$, or there exist a bipartite graph B in $\mathscr{B}(4p, p/2)$ such that $S = S_{32}(B)$ and the complement B' of B in $\mathscr{G}(4p, 7p/2 - 1)$ defined by

$$A(B') = \begin{bmatrix} J - I & J - N(B) \\ J - N(B)^{\mathrm{T}} & J - I \end{bmatrix}$$

is trace-minimal.

Furthermore, Eq. (14) *holds for all graphs G (or B') in $\mathscr{G}(4p, 7p/2 - 1)$.*

If $d = p/2$, $B \in \mathscr{B}(4p, p/2)$, and $B' \in \mathscr{G}(4p, 7p/2 - 1)$ is defined as above, then $\mathrm{spec}(S_{32}(B)) = \mathrm{spec}(S_{31}(B'))$.

With the help of Lemma 18, we now prove Theorem 7.

Proof of Theorem 7. Let $p/2 \leqslant d < p$, and G be a trace-minimal graph in $\mathscr{G}(4p, 3p + d - 1)$. By Lemma 18, $S = S_{31}(G)$ is a spectrum-maximal remainder matrix in

$\mathscr{M}(r)$. By Theorem 15, there exists a positive integer t_0 such that the class of design matrices $\mathscr{X}(S,t)$ is non-empty, balanced, and D-optimal for $t \geqslant t_0$. Let $X \in \mathscr{X}(S,t)$ and let $Y = L(X)$. Then by Lemma 11

$$\begin{aligned} G(nt+r,n) &= \det X^{\mathrm{T}}X \\ &= \frac{1}{t4^n}\det Y^{\mathrm{T}}Y \\ &= \frac{1}{t4^n}\det(4ptI_{4p}+S). \end{aligned}$$

Eq. (4) now follows from Eq. (14).

Note that if $d = p/2$ there are two possible kinds of spectrum-maximal remainder matrices $S \in \mathscr{M}(r)$. The first is $S = S_{31}(G)$ where $G \in \mathscr{G}(4p, 7p/2-1)$ is a trace-minimal graph. The other is $S = S_{32}(B)$ where $B \in \mathscr{B}(4p, p/2)$ and the complement graph $B' \in \mathscr{G}(4p, 7p/2-1)$ is trace-minimal. The second possibility does not always occur because it may happen that no B' is trace-minimal in $\mathscr{G}(4p, 7p/2-1)$. However, in the case where B' is a trace-minimal graph in $\mathscr{G}(4p, 7p/2-1)$, then $\operatorname{spec}(S_{31}(B')) = \operatorname{spec}(S_{32}(B))$ and hence Eq. (4) holds in case $d = p/2$.

Next let $0 \leqslant d < p/2$ and let B be a bipartite-trace-minimal graph in $\mathscr{B}(4p, d)$. By Lemma 18, $S = S_{32}(B)$ is a spectrum-maximal remainder matrix in $\mathscr{M}(r)$. By Theorem 15, there exists a positive integer t_0 such that the class of design matrices $\mathscr{X}(S,t)$ is non-empty, balanced, and D-optimal for all $t \geqslant t_0$. Let $X \in \mathscr{X}(S,t)$ and let $Y = L(X)$. Then by Lemma 11

$$\begin{aligned} G(nt+r,n) &= \det X^{\mathrm{T}}X \\ &= \frac{1}{t4^n}\det Y^{\mathrm{T}}Y \\ &= \frac{1}{t4^n}\det(4ptI_{4p}+S). \end{aligned}$$

Eq. (5) now follows from Eq. (15). □

4.4.4. $r \equiv 0 \pmod 4$

Let $r = 4d$. As in the case $r \equiv -1 \pmod 4$, the form of a spectrum-maximal remainder matrix in $\mathscr{M}(r)$ depends on whether $0 \leqslant d < p/2$, $p/2 < d \leqslant p$, or $d = p/2$. We need to define two types of matrices in $\mathscr{M}(r)$. Let G be a graph in $\mathscr{G}(4p, d)$ and define a matrix in $\mathscr{M}(r)$ by

$$S_{01}(G) := 4dI_{4p} - 4A(G). \tag{16}$$

Let B be a bipartite graph in $\mathscr{B}(4p, p+d)$ and define

$$S_{02}(B) := 4dI_{4p} + \begin{bmatrix} 0 & 2J_{2p} \\ 2J_{2p} & 0 \end{bmatrix} - 4A(B). \tag{17}$$

Lemma 19. *Let $r = 4d$ and suppose $S \in \mathscr{M}(r)$. If $0 \leqslant d < p/2$, then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exists a trace-minimal graph G in $\mathscr{G}(4p, d)$ such that $S = S_{01}(G)$.*

Furthermore, the following equation holds for all G in $\mathscr{G}(4p, d)$:

$$\det(4pt I_{4p} + S_{01}(G)) = 4^{4p}\mathrm{ch}_G(pt + d). \tag{18}$$

If $p/2 < d < p$, then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if there exists a bipartite-trace-minimal graph B in $\mathscr{B}(4p, p + d)$ such that $S = S_{02}(B)$.

Furthermore, the following equation holds for all bipartite graphs B in $\mathscr{B}(4p, p + d)$:

$$\det(4pt I_{4p} + S_{02}(B)) = \frac{4^{4p} t(pt + 2d)\mathrm{ch}_B(pt + d)}{(t - 1)(p(t + 1) + 2d)}.$$

If $d = p/2$ then S is spectrum-maximal in $\mathscr{M}(r)$ if and only if either there exists a trace-minimal graph G in $\mathscr{G}(4p, p/2)$ such that $S = S_{01}(G)$ or there exists a bipartite graph B in $\mathscr{B}(4p, 3p/2)$ such that $S = S_{02}(B)$ and the graph $B' \in \mathscr{G}(4p, p/2)$ defined by

$$A(B') = \begin{bmatrix} 0 & J - N(B) \\ J - N(B)^{\mathrm{T}} & 0 \end{bmatrix}$$

is trace-minimal.

Furthermore, Eq. (18) *holds for all G in $\mathscr{G}(4p, p/2)$.*

If $d = p/2$, $B \in \mathscr{B}(4p, 3p/2)$, and $B' \in \mathscr{G}(4p, p/2)$ is defined as above, then $\mathrm{spec}(S_{01}(B')) = \mathrm{spec}(S_{02}(B))$.

The proof of Theorem 8 is almost identical to the proof of Theorem 7 above.

It remains to prove Lemmas 12, 13, Theorem 15, and Lemmas 16–19, which will be done in Sections 5–7.

5. Proof of Lemmas 12 and 13

5.1. The module $\mathfrak{M}$

We begin by defining a $\mathbb{Z}$-module $\mathfrak{M}$. Let $S(4p, 2p) = \{v_1, \ldots, v_N\}$ be the set of all $4p$-tuples having $2p$ coordinates equal to 1 and $2p$ coordinates equal to -1. Then $N = \binom{4p}{2p}$. Let $\mathfrak{M}$ be the $\mathbb{Z}$-module generated by the $4p \times 4p$ symmetric integral matrices $\{vv^{\mathrm{T}} : v \in S(4p, 2p)\}$. Clearly if M is a matrix in $\mathfrak{M}$, then M is symmetric, each row of M sums to zero, and the entries on the main diagonal of M are the same. Only one additional property is necessary and sufficient for M to be in the module $\mathfrak{M}$:

Lemma 20. *Let $M = (M_{ij})$ be a symmetric $4p \times 4p$ integral matrix. Then $M \in \mathfrak{M}$ if and only if the following conditions are satisfied:*

(a) *the rows of M sum to zero*,
(b) *there exists an integer m such that $m_{ii} = m$ for all i*,
(c) $m_{is} + m_{it} + m_{js} + m_{jt} \equiv 0 \pmod 4$ *for all i, j, s, t.*

Furthermore, if M satisfies conditions (a) *and* (b), *then M satisfies condition* (c) *if and only if M is permutation similar to a blocked matrix.*

5.1.1. Proof of Lemma 20

Each of the generators vv^{T} of $\mathfrak{M}$ satisfies conditions (a)–(c) and thus every matrix $M \in \mathfrak{M}$ also satisfies these homogeneous linear conditions.

Next we show that if M satisfies conditions (a) and (b), then M satisfies (c) if and only if it is permutation similar to a blocked matrix. Let M be a symmetric integral matrix that satisfies conditions (a) and (b).

First suppose that P is a permutation matrix such that $P^{-1}MP$ is blocked. Since condition (c) is the same for M as it is for $P^{-1}MP$, we may assume that M is blocked. Let $1 \leqslant i, j, s, t \leqslant 4p$ and suppose that m_{is} and m_{it} are in the same block so that $m_{is} + m_{it} \equiv 2m \pmod 4$. Then m_{js} and m_{jt} are in the same block and so $m_{js} + m_{jt} \equiv 2m \pmod 4$. It follows that condition (c) holds. In case m_{is} and m_{it} are in different blocks, we have $m_{is} + m_{it} \equiv 2m + 2 \pmod 4$. But then m_{js} and m_{jt} are in different blocks and $m_{js} + m_{jt} \equiv 2m + 2 \pmod 4$. Again, condition (c) holds.

Conversely, suppose that condition (c) holds. Since $2m + 2m_{is} = m_{ii} + m_{is} + m_{si} + m_{ss} \equiv 0 \pmod 4$, all entries of M have the same parity as m. By performing a permutation similarity on M, we may assume that an integer k exists such that $m_{1s} \equiv m \pmod 4$ for $1 \leqslant s \leqslant k$ and $m_{1s} \equiv m + 2 \pmod 4$ for $k < s \leqslant 4p$. To see that M is blocked, suppose $1 \leqslant i, s \leqslant k$. Then $0 \equiv m_{11} + m_{1s} + m_{i1} + m_{is} \equiv 3m + m_{is} \pmod 4$. So $m_{is} \equiv m \pmod 4$; that is, all entries in the $k \times k$ upper left block of M are congruent to m modulo 4. For the upper right block, let $1 \leqslant i \leqslant k$ and $k < s \leqslant 4p$. Then $m_{1i} \equiv m \pmod 4$ and $m_{1s} \equiv m + 2 \pmod 4$. Thus $0 \equiv m_{11} + m_{1s} + m_{i1} + m_{is} \equiv 3m + 2 + m_{is} \pmod 4$. So $m_{is} \equiv m + 2 \pmod 4$. The argument for the other blocks is the same. Thus M is blocked. The fact that k is even follows from condition (b).

Now suppose that a matrix M satisfies conditions (a)–(c). We break the proof that $M \in \mathfrak{M}$ into two sublemmas.

Lemma 21. *Let M satisfy the three conditions in Lemma* 20. *Then there exist a matrix $M_0 \in \mathfrak{M}$ such that $M - M_0 \equiv 0 \pmod 4$ and each diagonal entry of $M - M_0$ is zero.*

Proof. Let M satisfy the conditions in Lemma 20. Since M is blocked, we assume that M is of the form of the block-matrix in (7), where the lower right block W is $2k \times 2k$ and $2k \leqslant 4p$. There are four cases: $m \equiv 0, 1, 2, 3 \pmod 4$.

We consider the case $m = 4q + 2 \equiv 2 \pmod 4$ first. Let a, b be non-negative integers with $a + b = 2p$ and define vectors $v_1, v_2 \in S(4p, 2p)$ as follows:

$$v_1 = [+e_a, \ -e_a, \ +e_b, \ -e_b],$$
$$v_2 = [+e_a, \ -e_a, \ -e_b, \ +e_b].$$

(e_a stands for the a-tuple of ones.) A direct calculation gives

$$M_2 := v_1 v_1^{\mathrm{T}} + v_2 v_2^{\mathrm{T}} = \begin{bmatrix} U_2 & V_2 \\ V_2^{\mathrm{T}} & W_2 \end{bmatrix},$$

where U_2 is a square matrix of size $2a \times 2a$, W_2 is a square matrix of size $2b \times 2b$, $U_2, W_2 \equiv 2 \pmod 4$, and $V_2 \equiv 0 \pmod 4$. Letting $a = 2p - k$ and $b = k$, we get the matrix M_2 such that $M - M_2 \equiv 0 \pmod 4$. Each main diagonal entry of $M - M_2$ equals $4q$. Letting v be any vector in $S(4p, 2p)$, we have $M_0 = M_2 + 4qvv^{\mathrm{T}} \in \mathfrak{M}$, $M - M_0 \equiv 0 \pmod 4$, and the main diagonal entries of $M - M_0$ are zero.

If $m = 4q \equiv 0 \pmod 4$, then take $M_0 = v_1 v_1^{\mathrm{T}} - v_2 v_2^{\mathrm{T}} + 4qvv^{\mathrm{T}} \in \mathfrak{M}$. Again $M - M_0 \equiv 0 \pmod 4$ and the diagonal entries of $M - M_0$ are zero.

The case $m = 4q + 3 \equiv 3 \pmod 4$ is a little more complicated. Let a, b, c, d, f, g, h be non-negative integers and define vectors v_1, v_2, v_3 as follows:

$$v_1 = [+e_a, \ +e_b, \ -e_c, \ -e_d, \ -e_f, \ +e_g, \ +e_h],$$
$$v_2 = [+e_a, \ -e_b, \ +e_c, \ -e_d, \ +e_f, \ -e_g, \ +e_h],$$
$$v_3 = [+e_a, \ -e_b, \ -e_c, \ +e_d, \ +e_f, \ +e_g, \ -e_h].$$

A direct calculation gives

$$M_3 := v_1 v_1^{\mathrm{T}} + v_2 v_2^{\mathrm{T}} + v_3 v_3^{\mathrm{T}} = \begin{bmatrix} U_3 & V_3 \\ V_3^{\mathrm{T}} & W_3 \end{bmatrix},$$

where U_3 is a square matrix of size $a + b + c + d$, W_3 is a square matrix of size $f + g + h$, $U_3, W_3 \equiv 3 \pmod 4$, and $V_3 \equiv 1 \pmod 4$. We will specify the parameters a, b, c, d, f, g, h satisfying

$$\begin{aligned} &a + b + c + d = 4p - 2k, \\ &f + g + h = 2k \end{aligned} \tag{19}$$

so that M_3 is $4p \times 4p$ and W_3 is $2k \times 2k$ and

$$\begin{aligned} &a + b - c - d - f + g + h = 0, \\ &a - b + c - d + f - g + h = 0, \\ &a - b - c + d + f + g - h = 0 \end{aligned} \tag{20}$$

so that $v_1, v_2, v_3 \in S(4p, 2p)$.

The choice of parameters depends on the congruence class of k modulo 3. Let $k = 3j + q$, where $q = 0$, 1 or 2. Choose

$$(a, b, c, d, f, g, h) = (p - 3j, p - j, p - j, p - j, 2j, 2j, 2j) + w_q,$$

where

$$w_0 = (0, 0, 0, 0, 0, 0, 0),$$
$$w_1 = (-1, -1, 0, 0, 0, 1, 1),$$
$$w_2 = (-2, 0, -1, -1, 2, 1, 1).$$

It is easy to verify that these choices for the parameters satisfy Eqs. (19) and (20). Thus we take $M_0 = M_3 + 4qvv^t$ so that $M - M_0 \equiv 0 \pmod 4$ and the main diagonal entries of $M - M_0$ are zero.

If $m = 4q + 1 \equiv 1 \pmod 4$ take $M_0 = -M_3 + 4(q+1)vv^t$. Again $M - M_0 \equiv 0 \pmod 4$, the main diagonal entries of $M - M_0$ are zero, and Lemma 21 is proved. □

The second lemma required for the proof of Lemma 20 is this.

Lemma 22. *Let $T = (t_{ij})$ be a symmetric $4p \times 4p$ integral matrix satisfying the following conditions*:

(a) *each row of T sums to zero*,
(b) $t_{ii} = 0$ *for all* i,
(c) $t_{ij} \equiv 0 \pmod 4$.

Then $T \in \mathfrak{M}$.

Proof. Suppose $T = (t_{ij})$ satisfies the three conditions. Define four vectors as follows:

$$v_1 = (+1,\ +1,\ -1,\ -1,\ u,\ -u),$$
$$v_2 = (+1,\ -1,\ +1,\ -1,\ u,\ -u),$$
$$v_3 = (-1,\ +1,\ -1,\ +1,\ u,\ -u),$$
$$v_4 = (-1,\ -1,\ +1,\ +1,\ u,\ -u),$$

where u is the $(2p-2)$-tuple consisting of all ones. Clearly $v_i \in S(4p, 2p)$ and a direct calculation gives

$$Q_2 := v_1v_1^{\mathrm{T}} - v_2v_2^{\mathrm{T}} - v_3v_3^{\mathrm{T}} + v_4v_4^{\mathrm{T}} = \begin{bmatrix} 0 & 4 & -4 & 0 \\ 4 & 0 & 0 & -4 \\ -4 & 0 & 0 & 4 \\ 0 & -4 & 4 & 0 \end{bmatrix} \oplus 0.$$

Clearly $Q_2 \in \mathfrak{M}$. By performing an appropriate permutation similarity on Q_2, we obtain a matrix $Q_i \in \mathfrak{M}$ having $+4$ in positions $(1, i)$, $(i, 1)$, $(2, i+1)$, $(i+1, 2)$ and -4 in positions $(1, i+1)$, $(i+1, 1)$, $(2, i)$, $(i, 2)$ and zeros elsewhere for each $3 \leqslant i \leqslant 4p-1$. Since each entry of T is divisible by 4, we have in particular that

$t_{1,2} = 4s_2$ for some integer s_2. Thus the $(1, 2)$ entry of the matrix $T_1 := T - s_2 Q_2$ is zero and T_1 satisfies the conditions in the lemma. The $(1, 3)$ entry of T_1 is divisible by 4 and hence there is an integer s_3 such that the $(1, 3)$ entry of $T_2 := T_1 - s_3 Q_3$ is zero and T_2 satisfies the conditions of the lemma. Inductively, there are integers s_i such that all entries in the first row (column) of $T - s_2 Q_2 - \cdots - s_{4p-1} Q_{4p-1}$ are zero except possibly the $(1, 4p)$ entry. But that entry must also be zero since the row sums of T, $Q_2, \ldots, Q_{4p-1}$ are zero. To summarize, there exists a matrix $Q \in \mathfrak{M}$ such that the first row (and column) of $T - Q$ is zero.

Arguing inductively on rows 2 to $4p - 3$ we have a matrix $Q \in \mathfrak{M}$ such that

$$T - Q = 0 \oplus \begin{bmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{bmatrix},$$

where a, b, c are integers. The row sums of T and Q are zero so $a = b = c = 0$. Thus $T = Q \in \mathfrak{M}$. $\square$

Now it is clear from Lemmas 21 and 22 that if M is a matrix satisfying conditions (a)–(c) of Lemma 20 then $M \in \mathfrak{M}$. The proof of Lemma 20 is complete.

5.1.2. *The matrix Y_0*

We need one more ingredient before embarking on the proofs of Lemmas 12 and 13. Let Y_0 be the $N \times 4p(\pm 1)$-matrix whose rows consist of all $(4p)$-tuples in $S(4p, 2p)$. It is not hard to show that $N = 2C(4p - 1)$ and that

$$\begin{aligned} \sum v_i v_i^{\mathrm{T}} &= Y_0^{\mathrm{T}} Y_0 \\ &= (N + 2C) I_{4p} - 2C J_{4p} \\ &= 2C(4pI - J), \end{aligned}$$

where $C = \frac{1}{2p}\binom{4p-2}{2p-1}$ is a Catalan number and hence an integer. For example, to compute the dot product of two distinct columns of Y_0, notice that they have the same sign in $2\binom{4p-2}{2p-2}$ coordinates and different signs in $2\binom{4p-2}{2p-1}$ coordinates. Thus all off-diagonal entries of $Y_0^{\mathrm{T}} Y_0$ equal

$$2\binom{4p-2}{2p-2} - 2\binom{4p-2}{2p-1} = -\frac{1}{p}\binom{4p-2}{2p-1} = -2C.$$

5.2. *Proof of Lemma 12*

Suppose S is a remainder matrix. Then there exist a non-negative integer t, a remainder $0 \leqslant r < n$, and $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$ such that Eq. (6) holds. Thus

$$Y = \begin{bmatrix} Y_1 \\ J_{t,4p} \end{bmatrix},$$

where Y_1 is a $((4p-1)t+r) \times 4p(\pm 1)$-matrix in which each row has $2p$ ones and $2p$ negative ones. Thus $Y^{\mathrm{T}}Y = Y_1^{\mathrm{T}}Y_1 + tJ_{4p,4p}$. Each row of Y_1 sums to zero. Thus each row of $Y_1^{\mathrm{T}}Y_1$ sums to zero, and so each row of $Y^{\mathrm{T}}Y$ sums to $4pt$. It follows that each row of S sums to zero.

Each diagonal entry of $Y^{\mathrm{T}}Y$ equals $4pt + r$. It follow that each diagonal entry of S is r.

Finally, to see that S is permutation similar to a blocked matrix, assume that the first u columns of Y have an even number of negative ones and the last w columns have an odd number of negative ones. Since the total number of negative ones in Y is even, u, w are even. Now suppose

$$S = \begin{bmatrix} U & V \\ V^{\mathrm{T}} & W \end{bmatrix},$$

where U is $u \times u$ and W is $w \times w$.

For each pair of integers $1 \leqslant i, j \leqslant 4p$ define a_{ij} to be the number of coordinates in which both the ith and jth columns of Y are 1, b_{ij} the number of coordinates in which the ith column is 1 and the jth column is -1, c_{ij} the number of coordinates in which the ith column is -1 and the jth column is 1, and d_{ij} the number of coordinates in which both the ith and jth columns are -1. Then

$$\begin{aligned}(Y^{\mathrm{T}}Y)_{ij} &= a_{ij} - b_{ij} - c_{ij} + d_{ij} \\ &\equiv (a_{ij} + b_{ij} + c_{ij} + d_{ij}) + 2(b_{ij} + d_{ij}) + 2(c_{ij} + d_{ij}) \pmod 4 \\ &\equiv r + 2(b_{ij} + d_{ij}) + 2(c_{ij} + d_{ij}) \pmod 4.\end{aligned}$$

If $0 \leqslant i, j \leqslant u$, then both $b_{ij} + d_{ij}$ and $c_{ij} + d_{ij}$ are even. Thus $U \equiv r \pmod 4$. If $u < i, j \leqslant 4p$, then both $b_{ij} + d_{ij}$ and $c_{ij} + d_{ij}$ are odd and so $W \equiv r \pmod 4$. If $1 \leqslant i \leqslant u < j \leqslant 4p$ then $b_{ij} + d_{ij}$ is even and $c_{ij} + d_{ij}$ is odd and thus $V \equiv r + 2 \pmod 4$.

Conversely, suppose that S satisfies the conditions of Lemma 12. Then $S \in \mathfrak{M}$. Thus $S = \sum x_i v_i v_i^{\mathrm{T}}$ for some integers x_i. Choose an integer y such that $y + x_i \geqslant 0$ for all i and let Y_1 be the matrix whose rows are the vectors v_i repeated $y + x_i$ times. Then

$$\begin{aligned}Y_1^{\mathrm{T}}Y_1 &= \sum (y + x_i) v_i v_i^{\mathrm{T}} \\ &= yY_0^{\mathrm{T}}Y_0 + S \\ &= 2Cy(4pI - J) + S.\end{aligned}$$

Then Y_1 has $2Cy(4p-1) + r$ rows. Append $t = 2Cy$ rows consisting of ones to Y_1 to get a matrix $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$. Then $Y^{\mathrm{T}}Y = 2Cy(4pI - J) + S + 2CyJ = 4ptI + S$. Thus S is a remainder matrix. The proof of Lemma 12 is complete.

5.3. Proof of Lemma 13

Let S be a remainder matrix with main diagonal entries equal to some r with $0 \leqslant r < 4p-1$. We show that $\mathscr{Y}(S,t)$ is non-empty for all sufficiently large t. The $4p \times 4p$ matrix $4pI - J$ satisfies the conditions of Lemma 20 and thus is in $\mathfrak{M}$. It follows that $q(4pI-J)+S \in \mathfrak{M}$ for every integer q and in particular for each $0 \leqslant q < 2C$. Indeed, for each $0 \leqslant q < 2C$, we have $q(4pI-J)+S = \sum x_i v_i v_i^{\mathrm{T}}$ for some integers x_i. Let y_q be an integer large enough that $y_q + x_i \geqslant 0$ for all i. Let Y_q be the matrix whose rows consists of the vectors v_i repeated $y_q + x_i$ times. Then the number of rows in Y_q is $\sum y_q + x_i = 2Cy_q(4p-1) + (4p-1)q + r$, and

$$\begin{aligned} Y_q^{\mathrm{T}} Y_q &= \sum (y_q + x_i) v_i v_i^{\mathrm{T}} \\ &= y_q \sum v_i v_i^{\mathrm{T}} + \sum x_i v_i v_i^{\mathrm{T}} \\ &= 2Cy_q(4pI - J) + q(4pI-J) + S \\ &= (2Cy_q + q)(4pI-J) + S. \end{aligned}$$

Let t_0 be the maximum value of $2Cy_q + q$ for $0 \leqslant q < 2C$ and suppose that $t \geqslant t_0$. We show that $\mathscr{Y}(S,t)$ is non-empty. Let $t = 2Cy + q$ for some $0 \leqslant q < 2C$ and suppose $t \geqslant t_0$. Then $y \geqslant y_q$. Let $Y^{\mathrm{T}} = \left[Y_0^{\mathrm{T}}, \ldots, Y_0^{\mathrm{T}}, Y_q^{\mathrm{T}}, J_{t,4p}{}^{\mathrm{T}}\right]$, where the matrix Y_0^{T} is repeated $y - y_q$ times. Then the number of rows in Y is $2C(4p-1)(y-y_q) + 2C(4p-1)y_q + (4p-1)q + r + t = 4pt + r$. The first $(4p-1)t + r$ rows are in $S(4p, 2p)$ and the last t rows consist of ones, so $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$.

To complete the proof, we must show that $Y^{\mathrm{T}}Y = 4ptI + S$:

$$\begin{aligned} Y^{\mathrm{T}}Y &= (y - y_q)Y_0^{\mathrm{T}}Y_0 + Y_q^{\mathrm{T}}Y_q + tJ \\ &= 2C(y-y_q)(4pI-J) + (2Cy_q + q)(4pI - J) + S + tJ \\ &= 4ptI + S. \end{aligned}$$

Thus $Y \in \mathscr{Y}(S,t)$, that is, $\mathscr{Y}(S,t)$ is non-empty and the proof of Lemma 13 is complete.

6. Proof of Theorem 15

We begin with an inequality about non-negative real numbers. Let λ be a multiset of $k > 1$ real numbers $w_1, \ldots, w_k$ satisfying $\sum w_i = s_1$ and $\sum w_i^2 = s_2$. It follows from the Cauchy-Schwarz inequality that $ks_2 - s_1^2 \geqslant 0$. Conversely, if s_1 and s_2 are real numbers with $ks_2 - s_1^2 \geqslant 0$, then there is a multiset whose sum is s_1 and sum of squares is s_2. In fact, there is such a multiset with only two distinct values, $\alpha(s_1,s_2) \leqslant \beta(s_1,s_2)$ where $\alpha(s_1,s_2)$ occurs with multiplicity $k-1$ and $\beta(s_1,s_2)$ with multiplicity one. That is there exist real numbers $\alpha(s_1,s_2) \leqslant \beta(s_1,s_2)$ such that

$$(k-1)\alpha(s_1,s_2) + \beta(s_1,s_2) = s_1, \quad (k-1)\alpha(s_1,s_2)^2 + \beta(s_1,s_2)^2 = s_2.$$

These essentially quadratic equations have two real solutions, but by choosing the plus/minus signs as follows:

$$\alpha(s_1, s_2) = \frac{(k-1)s_1 - \sqrt{(k-1)(ks_2 - s_1^2)}}{k(k-1)},$$

$$\beta(s_1, s_2) = \frac{s_1 + \sqrt{(k-1)(ks_2 - s_1^2)}}{k},$$

we get the desired two-valued multiset with $\alpha(s_1, s_2) \leqslant \beta(s_1, s_2)$. So $\{\overbrace{\alpha, \ldots, \alpha}^{k-1}, \beta\}$ is the required two-valued multiset, with $\alpha = \alpha(s_1, s_2)$, $\beta = \beta(s_1, s_2)$, described above. It is easy to see that if $s_1 \geqslant 0$ and $s_1^2 - s_2 \geqslant 0$, then $\alpha(s_1, s_2)$ is non-negative.

Now define a function

$$P(s_1, s_2) := \alpha(s_1, s_2)^{k-1}\beta(s_1, s_2) \tag{21}$$

on the region $ks_2 - s_1^2 \geqslant 0$. We record some properties of the function P in the next lemma.

Lemma 23. *Let $P(s_1, s_2)$ be the function defined by Eq.* (21) *on the region $ks_2 - s_1^2 \geqslant 0$. Then*

1. $\alpha(k\tau + s_1, k\tau^2 + 2\tau s_1 + s_2) = \tau + \alpha(s_1, s_2)$.
   $\beta(k\tau + s_1, k\tau^2 + 2\tau s_1 + s_2) = \tau + \beta(s_1, s_2)$.
2. $P(k\tau + s_1, k\tau^2 + 2\tau s_1 + s_2)$
   $= (\tau + \alpha(s_1, s_2))^{k-1}(\tau + \beta(s_1, s_2))$
   $= \tau^k + s_1\tau^{k-1} + \frac{1}{2}(s_1^2 - s_2)\tau^{k-2} + Q(s_1, s_2, \tau)$,
   for all real τ, where $Q(s_1, s_2, t)$ is a polynomial in t of degree $k-3$ whose coefficients depend only on s_1, s_2.
3. *$P(s_1, s_2)$ is decreasing in s_2, if $s_1^2 - s_2 \geqslant 0$, and $s_1 \geqslant 0$.*
4. *If $\lambda = \{w_1, \ldots, w_k\}$ is a multiset of k non-negative reals with $\sum w_i = s_1$ and $\sum w_i^2 = s_2$, then $\prod w_i \leqslant P(s_1, s_2)$.*

Proof. The last part of Lemma 23 was proved by Cohn [5].

To prove the third part, let

$$f(s_1, s_2) = \frac{1}{k-1}\sqrt{(k-1)(ks_2 - s_1^2)},$$

so that

$$\alpha(s_1, s_2) = \frac{s_1 - f(s_1, s_2)}{k}, \quad \beta(s_1, s_2) = \frac{s_1 + (k-1)f(s_1, s_2)}{k}.$$

Clearly, $f(s_1, s_2)$ is an increasing function of s_2. Now let

$$F(s_1, x) := (s_1 - x)^{k-1}(s_1 + (k-1)x).$$

It is easy to verify that if $0 \leqslant x \leqslant s_1$, then $\partial F/\partial x \leqslant 0$. But $0 \leqslant f(s_1, s_2) \leqslant s_1$ if and only if $s_1^2 - s_2 \geqslant 0$ and $s_1 \geqslant 0$. Thus $k^k P(s_1, s_2) = F(s_1, f(s_1, s_2))$ is a decreasing function of s_2.

To prove the first and second parts of the lemma, suppose that $ks_2 - s_1^2 \geqslant 0$, τ is a real number, $s_1' = k\tau + s_1$ and $s_2' = k\tau^2 + 2\tau s_1 + s_2$. Then $ks_2' - s_1'^2 = ks_2 - s_1^2$. Thus (s_1', s_2') is in the domain of P and $f(s_1', s_2') = f(s_1, s_2)$. It follows that

$$\alpha(s_1', s_2') = \tau + \alpha(s_1, s_2),$$
$$\beta(s_1', s_2') = \tau + \beta(s_1, s_2).$$

To complete the proof, expand

$$\begin{aligned}(\tau + \alpha)^{k-1}(\tau + \beta) &= \tau^k + ((k-1)\alpha + \beta)\tau^{k-1} + \biggl((k-1)\alpha\beta \\ &\quad + \frac{1}{2}(k-1)(k-2)\alpha^2\biggr)\tau^{k-2} + \cdots \\ &= \tau^k + s_1\tau^{k-1} + \frac{1}{2}(s_1^2 - s_2)\tau^{k-2} + \cdots,\end{aligned}$$

which follows since $(k-1)\alpha + \beta = s_1$ and $(k-1)\alpha^2 + \beta^2 = s_2$. □

Another technical lemma is needed, which is an application of Lemma 23 to the spectrum of a remainder matrix. Let $S \in \mathscr{M}(r)$ and define $s_1(S) = \mathrm{tr}(S)$ to be the sum of the eigenvalues of S and $s_2(S) = \mathrm{tr}(S^2)$ to be the sum of the squares of the eigenvalues of S.

Lemma 24. *Let S_0 be a remainder matrix in $\mathscr{M}(r)$. Then there exists a positive integer t_0 such that if $t \geqslant t_0$, $S \in \mathscr{M}(r)$, and $s_2(S) > s_2(S_0)$, then either $\mathscr{Y}(S, t)$ is empty or* $\det(4ptI_{4p} + S) < \det(4ptI_{4p} + S_0)$.

Proof. Assume that $S_0 \in \mathscr{M}(r)$. There exists an integer t_1 such that $4ptI_{4p} + S_0$ has positive eigenvalues for all $t \geqslant t_1$. Let $\tau = 4pt$. Since $2E_2(S_0) = (4pr)^2 - s_2(S_0)$, we have

$$\begin{aligned}\det(\tau I_{4p} + S_0) = \tau^{4p} + 4pr\tau^{4p-1} + \frac{1}{2}((4pr)^2 - s_2(S_0))\tau^{4p-2} \\ + q_1(S_0, t),\end{aligned} \tag{22}$$

where $q_1(S_0, t) = E_3(S_0)\tau^{4p-3} + \cdots + E_n(S_0)$ is a polynomial of degree $4p - 3$ with coefficients that depend only on S_0.

Since the set of integers $s_2(S)$ as $S \in \mathscr{M}(r)$ are non-negative, there exists $S_1 \in \mathscr{M}(r)$ such that $s_2(S_1)$ is minimal among all $s_2(S)$ for which $S \in \mathscr{M}(r)$ and $s_2(S) > s_2(S_0)$. That is, if $S \in \mathscr{M}(r)$ and $s_2(S) > s_2(S_0)$ then $s_2(S) \geqslant s_2(S_1) > s_2(S_0)$. There exists an integer t_2 such that $4ptI_{4p} + S_1$ has positive eigenvalues for all $t \geqslant t_2$. Let $t \geqslant t_2$ and $\tau = 4pt$. Then $(s_1(\tau I_{4p} + S_1), s_2(\tau I_{4p} + S_1))$ is in the domain of the function $P(s_1, s_2)$ and by Lemma 23 we have

$$P\big(s_1(\tau I_{4p}+S_1), s_2(\tau I_{4p}+S_1)\big) = \tau^{4p} + 4pr\tau^{4p-1} + \frac{1}{2}((4pr)^2 - s_2(S_1))\tau^{4p-2} + q_2(S_1,t), \tag{23}$$

where $q_2(S_1, t)$ is a polynomial of degree $4p - 3$ with coefficients depending only on S_1.

Since $s_2(S_1) > s_2(S_0)$, there exists an integer t_3 such that

$$\frac{1}{2}\big((4pr)^2 - s_2(S_1)\big)\tau^{4p-2} + q_2(S_1,t) < \frac{1}{2}\big((4pr)^2 - s_2(S_0)\big)\tau^{4p-2} + q_1(S_0,t) \tag{24}$$

if $t \geqslant t_3$.

Choose t_0 to be the maximum of t_1, t_2, t_3. Suppose that $t \geqslant t_0$, $S \in \mathscr{M}(r)$, and $s_2(S) > s_2(S_0)$. Then $s_2(S) \geqslant s_2(S_1)$ and $s_2(\tau I_{4p} + S) \geqslant s_2(\tau I_{4p} + S_1)$. If $\mathscr{Y}(S, t)$ is empty we are finished. If $Y \in \mathscr{Y}(S, t)$ for some Y then $Y^{\mathrm{T}}Y = 4pt I_{4p} + S$ has non-negative eigenvalues. Since the eigenvalues of $4pt I_{4p} + S$ are non-negative, $s_1(\tau I_{4p} + S)^2 - s_2(\tau I_{4p} + S) \geqslant 0$. Thus by Lemma 23 applied to $4pt I_{4p} + S$, we get

$$\begin{aligned}\det(\tau I_{4p}+S) &\leqslant P(s_1(\tau I_{4p}+S), s_2(\tau I_{4p}+S)) \\ &\leqslant P(s_1(\tau I_{4p}+S_1), s_2(\tau I_{4p}+S_1)).\end{aligned} \tag{25}$$

Combining inequalities (24) and (25) with Eqs. (23) and (22) we get $\det(\tau I_{4p} + S) < \det(\tau I_{4p} + S_0)$. □

Theorem 15 follows from the next result. To describe the notation $k(S)$ used in the next theorem, let S, S_0 be remainder matrices in $\mathscr{M}(r)$ and suppose S_0 is spectrum-maximal but S is not spectrum-maximal. By the definition of spectrum-maximal, there exists an integer $2 \leqslant k(S) \leqslant 4p$ such that $E_i(S) = E_i(S_0)$ for $i < k(S)$ and $E_i(S) < E_i(S_0)$ for $i = k(S)$.

Theorem 25. *Let $S_0 \in \mathscr{M}(r)$ be a spectrum-maximal remainder matrix and let $k(S)$ be defined on the $S \in \mathscr{M}(r)$ that are not spectrum-maximal as above. There exists an integer t_0 with the following properties*:

(a) *If $S \in \mathscr{M}(r)$ is not spectrum-maximal and $k(S) = 2$, then for all $t \geqslant t_0$ either $\mathscr{Y}(S, t)$ is empty or $\mathscr{Y}(S, t)$ is a non-D-optimal class.*
(b) *If $S \in \mathscr{M}(r)$ is not spectrum-maximal and $k(S) > 2$, then for all $t \geqslant t_0$ $\mathscr{Y}(S, t)$ is a non-empty non-D-optimal class.*
(c) *If $t \geqslant t_0$, then $\mathscr{Y}(S_0, t)$ is a non-empty D-optimal class.*

Proof. Let $S_0 \in \mathscr{M}(r)$ be a spectrum-maximal remainder matrix. Let t_2 be an integer such that $\mathscr{Y}(S_0, t)$ is non-empty for all $t \geqslant t_2$.

Proof of part (a). By Lemma 24, there exists an integer t_1 such that if $S \in \mathscr{M}(r)$ and $s_2(S) > s_2(S_0)$, then either $\mathscr{Y}(S, t)$ is empty or $\det(4ptI_{4p} + S) < \det(4ptI_{4p} + S_0)$. Now let t_a be the maximum of t_1, t_2 and suppose that $S \in \mathscr{M}(r)$ and $k(S) = 2$. Then $E_2(S) < E_2(S_0)$ and so $s_2(S) > s_2(S_0)$. If $\mathscr{Y}(S, t)$ is non-empty, there exists $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$ such that $Y^{\mathrm{T}}Y = 4ptI_{4p} + S$. Since $\mathscr{Y}(S_0, t)$ is also non-empty there exists $Y_0 \in \mathscr{C}(4pt + r, 4p, \pm 1)$ such that $Y_0^{\mathrm{T}}Y_0 = 4ptI_{4p} + S_0$. But then

$$\begin{aligned} \det Y^{\mathrm{T}}Y &= \det(4ptI_{4p} + S) \\ &< \det(4ptI_{4p} + S_0) \\ &= \det Y_0^{\mathrm{T}}Y_0. \end{aligned} \tag{26}$$

Hence Y is not D-optimal and $\mathscr{Y}(S, t)$ is a non-D-optimal class.

To prove part (b), let $\mathscr{M}_0(r)$ be the subset of remainder matrices S in $\mathscr{M}(r)$ that are not spectrum-maximal and for which $k(S) > 2$. Then $E_2(S) = E_2(S_0)$ and hence $s_2(S) = s_2(S_0)$ for all $S \in \mathscr{M}_0(r)$. Since S is an integral matrix on the ball $s_2(S) = s_2(S_0)$ for $S \in \mathscr{M}_0(r)$, it follows that $\mathscr{M}_0(r)$ is finite.

Let $\tau = 4pt$. We have

$$\det(\tau I + S) = \sum_k \tau^{4p-k} E_k(S),$$

and

$$\det(\tau I + S_0) = \sum_k \tau^{4p-k} E_k(S_0).$$

Since $E_i(S) = E_i(S_0)$ for $i < k(S)$,

$$\det(\tau I + S_0) - \det(\tau I + S)$$

is a polynomial in τ of degree $4p - k(S)$ and since $E_k(S) < E_k(S_0)$ for $k = k(S)$, the leading coefficient is positive. Hence there is a positive integer $t(S)$ such that if $t \geqslant t(S)$ then

$$\det(\tau I + S) < \det(\tau I + S_0)$$

for all $t \geqslant t(S)$. Let t_3 be the maximum value of $t(S)$ as S runs over the finite set $\mathscr{M}_0(r)$. It follows that if $t \geqslant t_3$ then $\det(\tau I + S) < \det(\tau I + S_0)$ for all $S \in \mathscr{M}_0(r)$.

Finally, for each $S \in \mathscr{M}_0(r)$ there exists an integer $t_4(S)$ such that if $t \geqslant t_4(S)$ then $\mathscr{Y}(S, t)$ is non-empty. Choose t_4 to be the maximum value of $t_4(S)$ as S runs over the finite set $\mathscr{M}_0(r)$. Let t_b be the maximum of t_2, t_3, t_4 and suppose $t \geqslant t_b$, $S \in \mathscr{M}(r)$ is not spectrum maximal, and $k(S) > 2$. Then $S \in \mathscr{M}_0(r)$, there exist $Y \in \mathscr{Y}(S, t)$, $Y_0 \in \mathscr{Y}(S_0, t)$, and

$$\begin{aligned} \det Y^{\mathrm{T}}Y &= \det(4ptI_{4p} + S) \\ &< \det(4ptI_{4p} + S_0) \\ &= \det Y_0^{\mathrm{T}}Y_0. \end{aligned} \tag{27}$$

Thus $\mathscr{Y}(S, t)$ is a non-D-optimal class.

Next we prove part (c). Let $t \geqslant t_a, t_b$. Then $\mathscr{Y}(S_0, t)$ is non-empty, say $Y_0 \in \mathscr{Y}(S_0, t)$. Suppose $Y \in \mathscr{C}(4pt + r, 4p, \pm 1)$ with $Y^{\mathrm{T}}Y = 4ptI_{4p} + S$ for some $S \in \mathscr{M}(r)$, that is, $Y \in \mathscr{Y}(S, t)$. We show that $\det Y^{\mathrm{T}}Y \leqslant \det Y_0^{\mathrm{T}}Y_0$. If S is spectrum-maximal, then $\det(4ptI_{4p} + S) = \det(4ptI_{4p} + S_0)$ and hence $\det Y^{\mathrm{T}}Y = \det Y_0^{\mathrm{T}}Y_0$. If S is not spectrum-maximal and $k(S) = 2$, then by Eq. (26) $\det Y^{\mathrm{T}}Y < \det Y_0^{\mathrm{T}}Y_0$, and if $k(S) > 2$, then by Eq. (27) $\det Y^{\mathrm{T}}Y < \det Y_0^{\mathrm{T}}Y_0$. □

Theorem 15 follows directly from Lemma 14 and Theorem 25.

7. Proofs of Lemmas 16–19

Let S, S_0 be remainder matrices in $\mathscr{M}(r)$ and suppose that S_0 is spectrum-maximal. By the definition of spectrum-maximal, $E_2(S) \leqslant E_2(S_0)$. And since $2E_2(M) = (\operatorname{tr} M)^2 - \operatorname{tr}(M^2)$ and $\operatorname{tr}(M^2) = \|M\|^2$ for any symmetric matrix M, and $\operatorname{tr}(S) = \operatorname{tr}(S_0) = 4pr$, we have $\|S_0\|^2 \leqslant \|S\|^2$. Thus we have the following lemma.

Lemma 26. *Let $S_0 \in \mathscr{M}(r)$ be a spectrum-maximal remainder matrix. Then $\|S_0\|^2 \leqslant \|S\|^2$ for all $S \in \mathscr{M}(r)$.*

In order to prove Lemmas 16–19, which characterize spectrum-maximal remainder matrices, we first characterize the *minimal-norm* remainder matrices. That is those $S_0 \in \mathscr{M}(r)$ for which $\|S_0\|^2 \leqslant \|S\|^2$ for all $S \in \mathscr{M}(r)$. The results in this section establish that all minimal-norm remainder matrices come from certain regular graphs on either $2p$ or $4p$ vertices. We also compute $\det(4ptI_{4p} + S)$ for each of the remainder matrices with minimal norm in terms of the characteristic polynomial of the adjacency matrix of the graph. These characterizations along with the determinant formulas will be used to establish Lemmas 16–19.

We use the following notation: the spectrum of the adjacency matrix $A(G)$ for a δ-regular graph G is denoted by $\operatorname{spec}(A(G))$. Since δ is always an eigenvalue of $A(G)$, we define and denote the *reduced spectrum* of $A(G)$ by $\operatorname{spec}'(A(G)) = \operatorname{spec}(A(G)) - \{\delta\}$. When G is connected, δ is a simple eigenvalue of $A(G)$ and thus $\operatorname{spec}'(A(G))$ does not contain δ. If B is a bipartite δ-regular graph, $\operatorname{spec}(A(B))$ is symmetric with respect to zero, that is $\operatorname{spec}(A(B)) = -\operatorname{spec}(A(B))$. Indeed, the eigenvalues of

$$A(B) = \begin{bmatrix} 0 & N(B) \\ N(B)^{\mathrm{T}} & 0 \end{bmatrix}$$

are of the form $\pm\lambda$ where λ is a singular value of $N(B)$. That is, the λ are the non-negative square roots of the eigenvalues of $N(B)^{\mathrm{T}}N(B)$. Since B is δ-regular, one of the singular values of $N(B)$ is δ. Denote the remaining singular values of $N(B)$ by $\operatorname{sing}'(N(B))$. Then the eigenvalues of $A(B)$ are $\pm\delta$ and $\pm\lambda$ as $\lambda \in \operatorname{sing}'(N(B))$.

We also need Newton's Identities [3], which when applied to the eigenvalues of a matrix X are

$$0 = \operatorname{tr}(X^q) - E_1(X)\operatorname{tr}(X^{q-1}) + E_2(X)\operatorname{tr}(X^{q-2}) - \cdots + (-1)^q q E_q(X). \quad (28)$$

7.1. $r \equiv 2 \pmod 4$

Let $r = 4d + 2$. Let G_1, G_2 be graphs in $\mathscr{G}(2p, p + d)$ and let $S_2(G_1, G_2)$ be the remainder matrix defined in Eq. (10). It is clear that $\|S_2(G_1, G_2)\|^2 = 4p(4d + 2)^2 + 32p^2 - 16p$. In the next lemma, we show that the minimal norm for matrices in $\mathscr{M}(r)$ is achieved only for remainder matrices of the form $S_2(G_1, G_2)$. We also express $\det(4ptI_{4p} + S_2(G_1, G_2))$ in terms of the characteristic polynomials of the adjacency matrices of G_1 and G_2, from which we establish Eq. (11) of Lemma 17.

Lemma 27. *Let $r = 4d + 2$ and suppose that $S \in \mathscr{M}(r)$. Then*

$$\|S\|^2 \geqslant 4p(4d + 2)^2 + 32p^2 - 16p, \quad (29)$$

with equality if and only if there exist graphs G_1, G_2 in $\mathscr{G}(2p, p + d)$ such that $S = S_2(G_1, G_2)$.

Furthermore,

$$\det(4ptI_{4p} + S_2(G_1, G_2)) = \frac{4^{4p}t^2 \operatorname{ch}_{G_1}(pt + d)\operatorname{ch}_{G_2}(pt + d)}{(t - 1)^2}. \quad (30)$$

Proof. Let $S \in \mathscr{M}(r)$ with

$$S = \begin{bmatrix} U & V \\ V^{\mathrm{T}} & W \end{bmatrix},$$

where U is a $u \times u$ matrix, W is a $w \times w$ matrix, $u + w = 4p$, $U, W \equiv 2 \pmod 4$ and $V \equiv 0 \pmod 4$. Then $\|U\|^2 \geqslant u(4d + 2)^2 + 4u(u - 1)$, with equality only if each off-diagonal entry of U is ± 2. Likewise, $\|W\|^2 \geqslant w(4d + 2)^2 + 4w(w - 1)$ with equality only if each off-diagonal entry of W is ± 2. Thus

$$\begin{aligned} \|S\|^2 &= \|U\|^2 + \|W\|^2 + 2\|V\|^2 \\ &\geqslant u(4d + 2)^2 + 4u(u - 1) + w(4d + 2)^2 + 4w(w - 1) \\ &= 4p(4d + 2)^2 + 4(u^2 + w^2) - 4(4p) \\ &\geqslant 4p(4d + 2)^2 + 4((2p)^2 + (2p)^2) - 16p \\ &= 4p(4d + 2)^2 + 32p^2 - 16p. \end{aligned}$$

The second inequality follows from the fact that $u^2 + w^2$ is minimal at $u = w = 2p$. Thus inequality (29) holds.

Inequality (29) is strict unless $u = w = 2p$, $V = 0$, and each off-diagonal entry of U and of W is ± 2. In that case $U = 4dI_{2p} + 2J_{2p} - 4A_1$, for some (0, 1)-matrix A_1. Since each row of U sums to zero, each row of A_1 contains exactly $d + p$ ones.

That is, $A_1 = A(G_1)$ for some graph G_1 in $\mathscr{G}(2p, p+d)$. Likewise $W = 4dI_{2p} + 2J_{2p} - 4A(G_2)$ for some graph G_2 in $\mathscr{G}(2p, p+d)$. Thus $S = S_2(G_1, G_2)$.

To prove Eq. (30), notice that

$$\begin{aligned} 4ptI_{4p} + S_2(G_1, G_2) = {} & [4(pt+d)I_{2p} + 2J_{2p} - 4A(G_1)] \\ & \oplus [4(pt+d)I_{2p} + 2J_{2p} - 4A(G_2)]. \end{aligned}$$

Since G_1 is $(p+d)$-regular,

$$\mathrm{ch}_{G_1}(x) = (x - (p+d)) \prod (x - \lambda)$$

and

$$\mathrm{ch}_{G_1}(pt+d) = p(t-1) \prod (pt + d - \lambda),$$

where the products are taken over $\lambda \in \mathrm{spec}'(A(G_1))$. It follows that the eigenvalues of $4dI_{2p} + 2J_{2p} - 4A(G_1)$ are 0, and $4(d-\lambda)$ where $\lambda \in \mathrm{spec}'(A(G_1))$. Thus

$$\begin{aligned} \det(4ptI_{2p} + 4dI_{2p} + 2J_{2p} - 4A(G_1)) &= 4pt \prod 4(pt + d - \lambda) \\ &= 4^{2p} pt \prod (pt + d - \lambda) \\ &= \frac{4^{2p} t \,\mathrm{ch}_{G_1}(pt+d)}{t-1}. \end{aligned}$$

A similar equality holds for G_2 and Eq. (30) follows. □

7.2. *Proof of Lemma 17: $r \equiv 2 \pmod 4$*

Let G_1, G_2 be trace-minimal graphs in $\mathscr{G}(2p, p+d)$, $S_0 = S_2(G_1, G_2)$, and let $S \in \mathscr{M}(r)$. We must show that $S \preceq S_0$.

From Lemma 27 we have $\|S\|^2 \geqslant \|S_0\|^2$ and thus $E_2(S) \leqslant E_2(S_0)$. If the inequality is strict, then $S \preceq S_0$ and we are finished. So assume that $\|S\|^2 = \|S_0\|^2$. Then by Lemma 27 there exist graphs H_1, H_2 in $\mathscr{G}(2p, p+d)$ such that $S = S_2(H_1, H_2)$. In the proof of Lemma 27 we showed that the eigenvalues of $S_2(H_1, H_2)$ are $0, 0, 4(d - h_1), 4(d - h_2)$ where $h_1 \in \mathrm{spec}'(A(H_1))$ and $h_2 \in \mathrm{spec}'(A(H_2))$. Thus

$$\begin{aligned} \mathrm{tr}(S^i) &= 4^i \left[\sum_{h_1} (d - h_1)^i + \sum_{h_2} (d - h_2)^i \right] \\ &= 4^i \sum_{j=0}^{i} \binom{i}{j} (-1)^j d^{i-j} \left[\sum_{h_1} h_1^j + \sum_{h_2} h_2^j \right] \qquad (31) \\ &= 4^i \sum_{j=0}^{i} \binom{i}{j} (-1)^j d^{i-j} \left[\mathrm{tr}(A(H_1)^j) + \mathrm{tr}(A(H_2)^j) - 2(p+d)^j \right], \end{aligned}$$

where the inner sums are taken over $h_1 \in \operatorname{spec}'(A(H_1))$ and $h_2 \in \operatorname{spec}'(A(H_2))$. Likewise

$$\operatorname{tr}(S_0^i) = 4^i \sum_{j=0}^{i} \binom{i}{j} (-1)^j d^{i-j} \left[\operatorname{tr}(A(G_1)^j) + \operatorname{tr}(A(G_2)^j) - 2(p+d)^j\right]. \tag{32}$$

Since G_1 is trace-minimal, either $\operatorname{spec}(A(H_1)) = \operatorname{spec}(A(G_1))$ or there exists a positive integer k_1 such that

$$\operatorname{tr}(A(G_1)^i) = \operatorname{tr}(A(H_1)^i) \quad \text{for } i < k_1,$$
$$\operatorname{tr}(A(G_1)^{k_1}) < \operatorname{tr}(A(H_1)^{k_1}).$$

A similar statement holds for G_2 and H_2. If $\operatorname{spec}(S) = \operatorname{spec}(S_0)$ then we are finished. If not, let k be the least positive integer for which either $\operatorname{tr}(A(G_1)^k) < \operatorname{tr}(A(H_1)^k)$ or $\operatorname{tr}(A(G_2)^k) < \operatorname{tr}(A(H_2)^k)$. Then from Eqs. (31) and (32) we have $\operatorname{tr}(S_0^i) = \operatorname{tr}(S^i)$ for $i < k$ and $(-1)^k \operatorname{tr}(S_0^k) < (-1)^k \operatorname{tr}(S^k)$. It follows from Newton's Identities (28) that $E_i(S_0) = E_i(S)$ for $i < k$ and $E_k(S) < E_k(S_0)$. Thus $S \preceq S_0$.

Conversely, suppose that $S \in \mathscr{M}(r)$ is a spectrum-maximal remainder matrix. By Lemma 26, S is a minimal-norm remainder matrix and by Lemma 27 there exist graphs H_1, H_2 in $\mathscr{G}(2p, p+d)$ such that $S = S_2(H_1, H_2)$. Now let G_1, G_2 be trace-minimal graphs in $\mathscr{G}(2p, p+d)$. By the first part of this lemma, $S_2(G_1, G_2)$ is spectrum-maximal. Since $S_2(H_1, H_2)$ is also spectrum-maximal, they have the same spectrum and hence $\operatorname{tr}(S_2(H_1, H_2)^i) = \operatorname{tr}(S_2(G_1, G_2)^i)$ for all i. If $\operatorname{tr}(A(H_1)^i) = \operatorname{tr}(A(G_1)^i)$ and $\operatorname{tr}(A(H_2)^i) = \operatorname{tr}(A(G_2)^i)$ for all i, then H_1 and H_2 are trace-minimal. Otherwise there is a least value of k for which either $\operatorname{tr}(A(G_1)^k) < \operatorname{tr}(A(H_1)^k)$ or $\operatorname{tr}(A(G_2)^k) < \operatorname{tr}(A(H_2)^k)$ then, arguing as above, we would have $E_k(S_2(H_1, H_2)) < E_k(S_2(G_1, G_2))$, contradicting the assumption that $S_2(H_1, H_2)$ is spectrum-maximal. It follows that H_1, H_2 are trace-minimal.

7.3. $r \equiv 1 \pmod 4$

Let $r = 4d + 1$, Let G_1, G_2 be graphs in $\mathscr{G}(2p, d)$ and let $S_1(G_1, G_2)$ be the remainder matrix defined in Eq. (8). Then $\|S_1(G_1, G_2)\|^2 = 4p(4d+1)^2 + 16p^2 + 32pd - 4p$ and this is the minimum norm for a matrix in $\mathscr{M}(r)$.

Lemma 28. *Let $r = 4d + 1$ and suppose that $S \in \mathscr{M}(r)$. Then*

$$\|S\|^2 \geqslant 4p(4d+1)^2 + 16p^2 + 32pd - 4p, \tag{33}$$

with equality if and only if the exist graphs G_1, G_2 in $\mathscr{G}(2p, d)$ such that $S = S_1(G_1, G_2)$.

Furthermore,

$$\det(4pt I_{4p} + S_1(G_1, G_2)) = \frac{4^{4p}(t+1)\operatorname{ch}_{G_1}(pt+d)\operatorname{ch}_{G_2}(pt+d)}{t}. \tag{34}$$

Proof. Let $S \in \mathscr{M}(r)$ and let $T = 4pI_{4p} - J_{4p} - S$. Then T satisfies the conditions in Lemma 12 and hence $T \in \mathscr{M}(4d' + 2)$, where $d' = p - d - 1$. It is easy to see that $\|S\|^2 = \|T\|^2 - 64p^3 + 48p^2 + 128p^2 d$. By Lemma 27 applied to T, we have

$$\|T\|^2 \geqslant 4p(4d' + 2)^2 + 32p^2 - 16p \tag{35}$$

and so

$$\begin{aligned}\|S\|^2 &\geqslant 4p(4d' + 2)^2 + 32p^2 - 16p - 64p^3 + 48p^2 + 128p^2 d\\ &= 4p(4d + 1)^2 + 16p^2 + 32pd - 4p.\end{aligned}$$

Now suppose that equality holds in inequality (33). Then equality holds in inequality (35) and by Lemma 27 there exist graphs G'_1, G'_2 in $\mathscr{G}(2p, p + d')$ such that $T = S_2(G'_1, G'_2)$. Let G_1, G_2 be the complements of G'_1, G'_2. Then G_1, G_2 are in $\mathscr{G}(2p, d)$ and $A(G'_i) = J_{2p} - I_{2p} - A(G_i)$. Thus

$$\begin{aligned}S &= 4pI_{4p} - J_{4p} - S_2(G'_1, G'_2)\\ &= 4pI_{4p} - J_{4p} - 4d'I_{4p} - \begin{bmatrix} 2J_{2p} - 4A(G'_1) & 0\\ 0 & 2J_{2p} - 4A(G'_2)\end{bmatrix}\\ &= 4dI_{4p} + \begin{bmatrix} J_{2p} - 4A(G_1) & -J_{2p}\\ -J_{2p} & J_{2p} - 4A(G_2)\end{bmatrix}\\ &= S_1(G_1, G_2).\end{aligned}$$

We now prove Eq. (34). Since G_1, G_2 are in $\mathscr{G}(2p, d)$, we have

$$\begin{aligned}\mathrm{ch}_{G_1}(x) &= (x - d)\prod(x - \lambda_1),\\ \mathrm{ch}_{G_1}(pt + d) &= pt\prod(pt + d - \lambda_1),\end{aligned}$$

where the products are taken over $\lambda_1 \in \mathrm{spec}'(A(G_1))$, and

$$\begin{aligned}\mathrm{ch}_{G_2}(x) &= (x - d)\prod(x - \lambda_2),\\ \mathrm{ch}_{G_2}(pt + d) &= pt\prod(pt + d - \lambda_2),\end{aligned}$$

where the products are taken over $\lambda_2 \in \mathrm{spec}'(A(G_2))$. Thus the eigenvalues of

$$S_1(G_1, G_2) = 4dI_{4p} + \begin{bmatrix} J_{2p} - 4A(G_1) & -J_{2p}\\ -J_{2p} & J_{2p} - 4A(G_2)\end{bmatrix}$$

are $0, 4p, 4(d - \lambda_1)$, and $4(d - \lambda_2)$, where $\lambda_1 \in \mathrm{spec}'(A(G_1))$ and $\lambda_2 \in \mathrm{spec}'(A(G_2))$. Thus

$$\det(4ptI_{4p} + S_1(G_1, G_2)) = (4pt)(4p(t+1)) \prod 4(pt + d - \lambda_1) \times \prod 4(pt + d - \lambda_2) = \frac{4^{4p}(t+1)\mathrm{ch}_{G_1}(pt+d)\mathrm{ch}_{G_2}(pt+d)}{t}. \qquad \square$$

7.4. *Proof of Lemma 16:* $r \equiv 1 \pmod 4$

Let G_1, G_2 be trace-minimal graphs in $\mathscr{G}(2p, d)$, $S_0 = S_1(G_1, G_2)$, and let $S \in \mathscr{M}(r)$. To prove that S_0 is spectrum-maximal we must show that $S \preceq S_0$.

From Lemma 28, we have $\|S\|^2 \geqslant \|S_0\|^2$ and thus $E_2(S) \leqslant E_2(S_0)$. If $E_2(S) < E_2(S_0)$, then we are finished. So assume that $E_2(S) = E_2(S_0)$. Then by Lemma 28 there exist graphs H_1, H_2 in $\mathscr{G}(2p, d)$ such that $S = S_1(H_1, H_2)$. In the proof of Lemma 28 we showed that the eigenvalues of $S_2(H_1, H_2)$ are $0, 4p, 4(d - h_1), 4(d - h_2)$ where $h_1 \in \mathrm{spec}'(A(H_1))$ and $h_2 \in \mathrm{spec}'(A(H_2))$. Thus

$$\begin{aligned}\mathrm{tr}(S^i) &= (4p)^i + 4^i \left[\sum_{h_1}(d-h_1)^i + \sum_{h_2}(d-h_2)^i\right] \\ &= (4p)^i + 4^i \sum_{j=0}^{i}\binom{i}{j}(-1)^j d^{i-j}\left[\sum_{h_1} h_1^j + \sum_{h_2} h_2^j\right] \qquad (36) \\ &= (4p)^i + 4^i \sum_{j=0}^{i}\binom{i}{j}(-1)^j d^{i-j}\left[\mathrm{tr}(A(H_1)^j) + \mathrm{tr}(A(H_2)^j) - 2d^j\right],\end{aligned}$$

where the inner sums are taken over $h_1 \in \mathrm{spec}'(A(H_1))$ and $h_2 \in \mathrm{spec}'(A(H_2))$. Likewise

$$\mathrm{tr}(S_0^i) = (4p)^i + 4^i \sum_{j=0}^{i}\binom{i}{j}(-1)^j d^{i-j} \times \left[\mathrm{tr}(A(G_1)^j) + \mathrm{tr}(A(G_2)^j) - 2d^j\right]. \qquad (37)$$

Since G_1 is trace-minimal, either $\mathrm{spec}(A(H_1)) = \mathrm{spec}(A(G_1))$ or there exists a positive integer k_1 such that

$$\mathrm{tr}(A(G_1)^i) = \mathrm{tr}(A(H_1)^i) \quad \text{for } i < k_1$$
$$\mathrm{tr}(A(G_1)^{k_1}) < \mathrm{tr}(A(H_1)^{k_1}).$$

A similar statement holds for G_2 and H_2. If $\mathrm{spec}(A(H_q)) = \mathrm{spec}(A(G_q))$ for $q = 1, 2$, then $\mathrm{spec}(S) = \mathrm{spec}(S_0)$ and we are finished. If not, let k be the least positive integer for which either $\mathrm{tr}(A(G_1)^k) < \mathrm{tr}(A(H_1)^k)$ or $\mathrm{tr}(A(G_2)^k) < \mathrm{tr}(A(H_2)^k)$. Then $\mathrm{tr}(A(G_1)^i) = \mathrm{tr}(A(H_1)^i)$ and $\mathrm{tr}(A(G_2)^i) = \mathrm{tr}(A(H_2)^i)$, for $i < k$. In view of Eqs. (36) and (37), it follows that $\mathrm{tr}(S^i) = \mathrm{tr}(S_0^i)$ for $i < k$ and $(-1)^k\mathrm{tr}(S_0^k) < (-1)^k\mathrm{tr}(S^k)$. Since $\mathrm{tr}(S^i) = \mathrm{tr}(S_0^i)$ for $i < k$, it follows from Newton's Identities (28) that $E_i(S) = E_i(S_0)$ for $i < k$. And since $(-1)^k\mathrm{tr}(S_0^k) < (-1)^k\mathrm{tr}(S^k)$, we have $E_k(S) < E_k(S_0)$.

Conversely, suppose that $S \in \mathscr{M}(r)$ is a spectrum-maximal remainder matrix. By Lemma 26, S is a minimal-norm remainder matrix and by Lemma 28 there exist graphs H_1, H_2 in $\mathscr{G}(2p, d)$ such that $S = S_1(H_1, H_2)$. Now let G_1, G_2 be trace-minimal graphs in $\mathscr{G}(2p, d)$. By the first part of this Lemma, $S_1(G_1, G_2)$ is spectrum-maximal. Since $S_1(H_1, H_2)$ is also spectrum-maximal, they have the same spectrum and hence $\mathrm{tr}(S_1(H_1, H_2)^i) = \mathrm{tr}(S_1(G_1, G_2)^i)$ for all i. If $\mathrm{tr}(A(H_1)^i) = \mathrm{tr}(A(G_1)^i)$ and $\mathrm{tr}(A(H_2)^i) = \mathrm{tr}(A(G_2)^i)$ for all i, then H_1 and H_2 are trace-minimal. Otherwise there is a least value of k for which either $\mathrm{tr}(A(G_1)^k) < \mathrm{tr}(A(H_1)^k)$ or $\mathrm{tr}(A(G_2)^k) < \mathrm{tr}(A(H_2)^k)$. Then, arguing as above, we would have $E_k(S_1(H_1, H_2)) < E_k(S_1(G_1, G_2))$, contradicting the assumption that $S_1(H_1, H_2)$ is spectrum-maximal. It follows that H_1, H_2 are trace-minimal.

Finally, Eq. (9) has been proved in the proof of Lemma 28.

7.5. $r \equiv 0 \pmod 4$

Let $r = 4d$. The minimum norm for a matrix in $\mathscr{M}(r)$ depends on whether $0 \leqslant d \leqslant p/2$ or $p/2 \leqslant d \leqslant p$. Let G be a graph in $\mathscr{G}(4p, d)$ and let $S_{01}(G)$ be the remainder matrix in $\mathscr{M}(r)$ defined in Eq. (16). Then $\|S_{01}(G)\|^2 = 4p(4d)^2 + 64pd$. The other remainder matrix $S_{02}(B) \in \mathscr{M}(r)$, defined in Eq. (17), comes from a bipartite graph B in $\mathscr{B}(4p, p + d)$. Its norm is given by $\|S_{02}(B)\|^2 = 4p(4d)^2 + 32p^2$. It is easy to check that $S_{01}(G)$ has the smaller norm if $0 \leqslant d < p/2$ and that $S_{02}(B)$ has the smaller norm if $p/2 < d \leqslant p$. If p is even and $d = p/2$, then the norms are equal.

Lemma 29. *Let $r = 4d$ and suppose $S \in \mathscr{M}(r)$. If $0 \leqslant d < p/2$, then*

$$\|S\|^2 \geqslant 4p(4d)^2 + 64pd,$$

with equality if and only if there exists a graph G in $\mathscr{G}(4p, d)$ such that $S = S_{01}(G)$.

Furthermore,

$$\det(4ptI_{4p} + S_{01}(G)) = 4^{4p}\mathrm{ch}_G(pt + d). \tag{38}$$

If $p/2 < d < p$, then

$$\|S\|^2 \geqslant 4p(4d)^2 + 32p^2,$$

with equality if and only if there exists a bipartite graph B in $\mathscr{B}(4p, p + d)$ such that $S = S_{02}(B)$.

Furthermore,

$$\det(4ptI_{4p} + S_{02}(B)) = \frac{4^{4p}t(pt + 2d)\mathrm{ch}_B(pt + d)}{(t - 1)(p(t + 1) + 2d)}. \tag{39}$$

If p is even and $d = p/2$, then

$$\|S\|^2 \geqslant 4p(4d)^2 + 64pd = 4p(4d)^2 + 32p^2,$$

with equality if and only if either there exists a graph G in $\mathscr{G}(4p, p/2)$ such that $S = S_{01}(G)$ or there exists a bipartite graph B in $\mathscr{B}(4p, 3p/2)$ such that $S = S_{02}(B)$.

Proof. Let $S \in \mathscr{M}(r)$ with

$$S = \begin{bmatrix} U & V \\ V^{\mathrm{T}} & W \end{bmatrix},$$

where U is a $u \times u$ matrix, W is a $w \times w$ matrix, $u + w = 4p$, $U, W \equiv 0 \pmod 4$ and $V \equiv 2 \pmod 4$. Assume, without loss of generality, that $u \leqslant 2p$. Let $\sum(P)$ denote the sum of all entries in the matrix P and $\sum_{\text{off}}(P)$ the sum of all off-diagonal entries of P. Since the row sums of S are zero, $\sum_{\text{off}}(U) + 4du = \sum(U) = -\sum(V) = \sum(W) = \sum_{\text{off}}(W) + 4dw$. Thus $\sum_{\text{off}}(U) - \sum_{\text{off}}(W) = 4d(w-u) = 4d(4p-2u)$. Let $|U|$ be the matrix whose entries are $|U_{i,j}|$ and $|U|^{(2)}$ the matrix whose entries are $|U_{i,j}|^2$. Then

$$\begin{aligned}\sum_{\text{off}}\left(|U|^{(2)}\right) + \sum_{\text{off}}\left(|W|^{(2)}\right) &\geqslant 4\left(\sum_{\text{off}}(|U|) + \sum_{\text{off}}(|W|)\right)\\ &\geqslant 4\left(\sum_{\text{off}}(U) - \sum_{\text{off}}(W)\right)\\ &= 16d(w-u),\end{aligned}$$

with equality if and only if all non-zero off-diagonal entries of U are 4 and all non-zero off-diagonal entries of W are -4. Thus

$$\begin{aligned}\|S\|^2 &= \|U\|^2 + \|W\|^2 + 2\|V\|^2\\ &= 4p(4d)^2 + \sum_{\text{off}}\left(|U|^{(2)}\right) + \sum_{\text{off}}\left(|W|^{(2)}\right) + 2\|V\|^2\\ &\geqslant 4p(4d)^2 + 16d(w-u) + 2uw(\pm 2)^2\\ &= 4p(4d)^2 + 16d(4p-2u) + 8uw\\ &= 4p(4d)^2 + 64pd + 8[4(p-d)u - u^2],\end{aligned}$$

with equality if and only if all non-zero off-diagonal entries of U are 4, all non-zero off-diagonal entries of W are -4, and each off-diagonal entry of V is ± 2. The graph of the function $f(u) = 4(p-d)u - u^2$ is a parabola with vertex at $(2(p-d), 4(p-d)^2)$. Thus $f(u)$ attains its minimum value on the interval $0 \leqslant u \leqslant 2p$ at one of the end points, either $u = 0$ or $u = 2p$. There are three cases.

First suppose $0 \leqslant d < p/2$, then $p < 2(p-d)$ so $f(u)$ is minimal at $u = 0$. Thus $\|S\|^2 \geqslant 4p(4d)^2 + 64pd$, with equality if and only if $S = W$ (since $u = 0$), and each non-zero off-diagonal entry of S is -4. Since the diagonal entries of S are

$4d$, and each row of S sums to zero, there are exactly d non-zero off-diagonal entries in each row of S. That is $S = S_{01}(G)$ for some graph G in $\mathscr{G}(4p, d)$.

We now prove Eq. (38). Since G is a d-regular graph,

$$\mathrm{ch}_G(x) = (x - d) \prod (x - \lambda)$$

and

$$\mathrm{ch}_G(pt + d) = pt \prod (pt + d - \lambda),$$

where the products are taken over $\lambda \in \mathrm{spec}'(A(G))$. It follows that the eigenvalues of $S_{01}(G)$ are 0 and $4d - 4\lambda$ as $\lambda \in \mathrm{spec}'(A(G))$. Thus

$$\begin{aligned}\det(4ptI_{4p} + S_{01}(G)) &= 4pt \prod (4pt + 4d - 4\lambda)\\ &= 4^{4p} pt \prod (pt + d - \lambda)\\ &= 4^{4p} \mathrm{ch}_G(pt + d).\end{aligned}$$

Second suppose that $p/2 < d \leqslant p$. Then $2(p - d) < p$ so $f(u)$ is minimal at $u = 2p$. Thus $\|S\|^2 \geqslant 4p(4d)^2 + 64pd + 8f(2p) = 4p(4d)^2 + 32p^2$, with equality if and only if $u = w = 2p$, each non-zero off-diagonal entry of U is 4, each non-zero off-diagonal entry of W is -4, and all entries of V are ± 2. Now since $\sum(U) = \sum(W)$, all off-diagonal entries of both U and W are zero. Thus each row and each column of V sums to $-4d$. Thus each row and each column of V contains exactly $p - d$ entries equal to 2 and $p + d$ entries equal to -2. It follows that $V = 2J_{2p} - 4N$ where N is a (0, 1)-matrix having exactly $p + d$ ones in each row and each column. To summarize,

$$S = 4dI_{4p} + \begin{bmatrix} 0 & 2J_{2p} - 4N \\ 2J_{2p} - 4N^{\mathrm{T}} & 0 \end{bmatrix}.$$

Now let B be the bipartite graph in $\mathscr{B}(4p, p + d)$ such that $N(B) = N$. That is

$$A(B) = \begin{bmatrix} 0 & N \\ N^{\mathrm{T}} & 0 \end{bmatrix} = \begin{bmatrix} 0 & N(B) \\ N(B)^{\mathrm{T}} & 0 \end{bmatrix}.$$

Then $S = S_{02}(B)$.

We now prove Eq. (39). The eigenvalues of $A(B)$ are $\pm(d + p)$ and $\pm\lambda$ as $\lambda \in \mathrm{sing}'(N(B))$. Thus

$$\mathrm{ch}_B(x) = (x - (p + d))(x + (p + d)) \prod (x - \lambda)(x + \lambda),$$

where the product is taken over $\lambda \in \mathrm{sing}'(N(B))$. Thus

$$\mathrm{ch}_B(pt + d) = p(t - 1)(p(t + 1) + 2d) \prod (pt + d - \lambda)(pt + d + \lambda).$$

It follows that the eigenvalues of

$$S_{02}(B) = 4dI_{4p} + \begin{bmatrix} 0 & 2J_{2p} \\ 2J_{2p} & 0 \end{bmatrix} - 4A(B)$$

are 0, $8d$, and $4d \pm 4\lambda$, where $\lambda \in \operatorname{sing}'(N(B))$. Hence

$$\begin{aligned}\det(4ptI_{4p} + S_{02}(B)) &= 4pt(4pt + 8d)\prod(4pt + 4d - 4\lambda)(4pt + 4d + 4\lambda)\\ &= 4^{4p}pt(pt + 2d)\prod(pt + d - \lambda)(pt + d + \lambda)\\ &= \frac{4^{4p}t(pt + 2d)\mathrm{ch}_B(pt + d)}{(t-1)(p(t+1) + 2d)}.\end{aligned}$$

Third and finally, suppose that $d = p/2$. Then $p = 2(p - d)$ and so $f(u)$ is minimal at both $u = 0$ and $u = 2p$. Arguing as in the previous cases we see that either $S = S_{01}(G)$ for some graph G in $\mathscr{G}(4p, p/2)$ or $S = S_{02}(B)$ for some bipartite graph B in $\mathscr{B}(4p, 3p/2)$. $\square$

7.6. *Proof of Lemma 19: $r \equiv 0 \pmod 4$*

Let $0 \leqslant d < p/2$, G be a trace-minimal graph in $\mathscr{G}(4p, d)$, $S_0 = S_{01}(G)$, and $S \in \mathscr{M}(r)$. To prove that S is spectrum-maximal, we must show that $S \preceq S_0$. From Lemma 29 we have $\|S\|^2 \geqslant \|S_0\|^2$ and thus $E_2(S) \leqslant E_2(S_0)$. If $E_2(S) < E_2(S_0)$ then we are finished. So assume that $E_2(S) = E_2(S_0)$. Then by Lemma 29, there exists a graph H in $\mathscr{G}(4p, d)$ such that $S = S_{01}(H)$.

The eigenvalues of $S_{01}(H)$ are 0 and $4(d - h)$, where $h \in \operatorname{spec}'(A(H))$. Thus

$$\begin{aligned}\operatorname{tr}(S_{01}(H)^i) &= \sum_h [4(d-h)]^i\\ &= 4^i \sum_{j=0}^{i} \binom{i}{j} (-1)^j d^{i-j} \sum_h h^j\\ &= 4^i \sum_j \binom{i}{j} d^{i-j} (-1)^j [\operatorname{tr}(A(H)^j) - d^j]. \qquad (40)\end{aligned}$$

Likewise

$$\operatorname{tr}(S_{01}(G)^i) = 4^i \sum_j \binom{i}{j} d^{i-j} (-1)^j [\operatorname{tr}(A(G)^j) - d^j].$$

If $\operatorname{spec}(A(H)) = \operatorname{spec}(A(G))$ then $\operatorname{spec}(S) = \operatorname{spec}(S_0)$ and we are finished. If not, let $3 \leqslant k \leqslant 4p$ be an integer such that $\operatorname{tr}(A(H)^i) = \operatorname{tr}(A(G)^i)$ for $i < k$ and $\operatorname{tr}(A(G)^k) < \operatorname{tr}(A(H)^k)$. It follows from Eq. (40) that $\operatorname{tr}(S^i) = \operatorname{tr}(S_0^i)$ for $i < k$ and $(-1)^k\operatorname{tr}(S_0^k) < (-1)^k\operatorname{tr}(S^k)$. Thus from Newton's Identities (28) we have $E_k(S) < E_k(S_0)$ and we are finished.

Let $p/2 < d < p$, B be a bipartite-trace-minimal graph in $\mathscr{B}(4p, p + d)$, $S_0 = S_{02}(B)$, and $S \in \mathscr{M}(r)$. We must show that $S \preceq S_0$. From Lemma 29 we have $\|S\|^2 \geqslant$

$\|S_0\|^2$. If the inequality is strict, then $E_2(S) < E_2(S_0)$ and we are finished. So assume that $\|S\|^2 = \|S_0\|^2$. Then by Lemma 29 there exists a bipartite graph H in $\mathscr{B}(4p, p+d)$ such that $S = S_{02}(H)$. Then

$$\mathrm{ch}_H(x) = (x-(p+d))(x+(p+d))\prod(x-\lambda)(x+\lambda),$$

where the product is taken over $\lambda \in \mathrm{sing}'(N(H))$. The eigenvalues of $S_{02}(H)$ are 0, $8d$, and $4(d \pm \lambda)$ where $\lambda \in \mathrm{sing}'(N(H))$. Thus

$$\begin{aligned}\mathrm{tr}(S_{02}(H)^i) &= (8d)^i + \sum_\lambda [4(d+\lambda)]^i + [4(d-\lambda)]^i \\ &= (8d)^i + 4^i \sum_\lambda \sum_{j=0}^{i} \binom{i}{j} [d^{i-j}\lambda^j + d^{i-j}(-\lambda)^j] \\ &= (8d)^i + 4^i \sum_j \binom{i}{j} d^{i-j} \sum_\lambda [\lambda^j + (-\lambda)^j] \\ &= (8d)^i + 4^i \sum_j \binom{i}{j} d^{i-j} [\mathrm{tr}(A(H)^j) - ((d+p)^j + (-(d+p))^j)].\end{aligned}$$

Likewise

$$\begin{aligned}\mathrm{tr}(S_{02}(B)^i) = (8d)^i + 4^i \sum_j \binom{i}{j} d^{i-j} \\ \times [\mathrm{tr}(A(B)^j) - ((d+p)^j + (-(d+p))^j)].\end{aligned}$$

If $\mathrm{spec}(A(H)) = \mathrm{spec}(A(B))$ then $\mathrm{spec}(S_{02}(H)) = \mathrm{spec}(S_{02}(B))$ and we are finished. If not, since B is bipartite-trace-minimal, there exists $4 \leqslant k \leqslant 2p$ such that $\mathrm{tr}(A(H)^{2i}) = \mathrm{tr}(A(B)^{2i})$ for $i < k$ and $\mathrm{tr}(A(B)^{2k}) < \mathrm{tr}(A(H)^{2k})$. It follows from the above formulas for $\mathrm{tr}(S_{02}(B)^i)$ and $\mathrm{tr}(S_{02}(H)^i)$ that $\mathrm{tr}(S_{02}(B)^i) = \mathrm{tr}(S_{02}(H)^i)$ for $i < 2k$ and $\mathrm{tr}(S_{02}(B)^{2k}) < \mathrm{tr}(S_{02}(H)^{2k})$. Thus by Newton's Identities (28) with $q \leqslant 2k$ we have $E_i(S_{02}(H)) = E_i(S_{02}(B))$ for $i < 2k$ and $E_{2k}(S_{02}(H)) < E_{2k}(S_{02}(B))$ and we are finished.

Finally, the proof of the case $d = p/2$ is based on the following observation: if $B \in \mathscr{B}(4p, 3p/2)$ and B' is the graph whose adjacency matrix is

$$A(B') = \begin{bmatrix} 0 & J - N(B) \\ J - N(B)^{\mathrm{T}} & 0 \end{bmatrix}, \tag{41}$$

then

$$\mathrm{spec}(S_{02}(B)) = \mathrm{spec}(S_{01}(B')). \tag{42}$$

Indeed, write $S_{01}(B') = 4dI_{4p} + T_1$ and $S_{02}(B) = 4dI_{4p} + T_2$, where

$$T_1 = \begin{bmatrix} 0 & -4J + 4N(B) \\ -4J + 4N(B)^{\mathrm{T}} & 0 \end{bmatrix},$$

$$T_2 = \begin{bmatrix} 0 & 2J - 4N(B) \\ 2J - 4N(B)^{\mathrm{T}} & 0 \end{bmatrix}.$$

Clearly $\mathrm{tr}(T_1^i) = \mathrm{tr}(T_2^i) = 0$ if i is odd. Thus it suffices to show that $T_1^2 = T_2^2$. Direct calculations give $T_1^2 = M_1 \oplus M_1^{\mathrm{T}}$, where

$$\begin{aligned} M_1 &= (-4J + 4N(B)^{\mathrm{T}})(-4J + 4N(B)) \\ &= 16(-J + N(B)^{\mathrm{T}})(-J + N(B)) \\ &= 16(-pJ + N(B)^{\mathrm{T}} N(B)). \end{aligned}$$

The last equality follows from the fact that $N(B)$ has $3p/2$ ones in each row and column. A similar calculation gives $T_2^2 = M_2 \oplus M_2^{\mathrm{T}}$, where

$$\begin{aligned} M_2 &= (2J - 4N(B)^{\mathrm{T}})(2J - 4N(B)) \\ &= 4(J - 2N(B)^{\mathrm{T}})(J - 2N(B)) \\ &= 16(-pJ + N(B)^{\mathrm{T}} N(B)). \end{aligned}$$

Again, the last equality follows from the fact that $N(B)$ has $3p/2$ ones in each row and column. Thus $M_1 = M_2$, $T_1^2 = T_2^2$, $\mathrm{spec}(T_1) = \mathrm{spec}(T_2)$, and so Eq. (42) holds.

Now suppose G is a trace-minimal graph in $\mathscr{G}(4p, p/2)$. We show that $S_{01}(G)$ is spectrum-maximal in $\mathscr{M}(r)$.

Let $S \in \mathscr{M}(r)$. If $\|S\|^2 > \|S_{01}(G)\|^2$ we are finished since this implies that $E_2(S) < E_2(S_{01}(G))$. If $\|S\|^2 = \|S_{01}(G)\|^2$ then by Lemma 29 either $S = S_{01}(H)$ for some $H \in \mathscr{G}(4p, p/2)$ or $S = S_{02}(B)$ for some $B \in \mathscr{B}(4p, 3p/2)$. In the first case, use the same argument as in the case $0 \leqslant d < p/2$ to get $S_{01}(H) \preceq S_{01}(G)$. For the second case, let $B' \in \mathscr{G}(4p, p/2)$ be the graph defined by Eq. (41). As before, with $H = B'$, we have $S_{01}(B') \preceq S_{01}(G)$. Thus by Eq. (42), $S_{02}(B) \preceq S_{01}(G)$.

To finish the case $d = p/2$, we now assume that $B \in \mathscr{B}(4p, 3p/2)$ is a bipartite graph such that the graph B' defined in Eq. (41) is trace-minimal. By the previous argument, $S_{01}(B')$ is spectrum-maximal in $\mathscr{M}(r)$, and thus by Eq. (42), $S_{02}(B)$ is spectrum-maximal in $\mathscr{M}(r)$.

We now prove the converse of Lemma 19. Suppose $0 \leqslant d < p/2$ and that $S \in \mathscr{M}(r)$ is spectrum-maximal. Let G be a trace-minimal graph in $\mathscr{G}(4p, d)$. By the first part of the proof, $S_{01}(G)$ is spectrum-maximal. It follows that $\mathrm{spec}(S) = \mathrm{spec}(S_{01}(G))$, since all spectrum-maximal remainder matrices in $\mathscr{M}(r)$ have the same spectrum. In particular $\|S\|^2 = \|S_{01}(G)\|^2$ and thus by Lemma 29 there exists a graph $H \in \mathscr{G}(d, 4p)$ such that $S = S_{01}(H)$. Thus $\mathrm{spec}(S_{01}(H)) = \mathrm{spec}(S_{01}(G))$ and hence $\mathrm{spec}(A(H)) = \mathrm{spec}(A(G))$. It follows that H is trace-minimal.

The argument for the converse in the case, $p/2 < d < p$ is similar.

Now suppose $d = p/2$ and $S \in \mathscr{M}(r)$ is spectrum-maximal. Let G be a trace-minimal graph in $\mathscr{G}(4p, p/2)$. As in the previous case, it follows that $\mathrm{spec}(S) = \mathrm{spec}(S_{01}(G))$ and $\|S\|^2 = \|S_{01}(G)\|^2$. Thus by Lemma 29, either there exists a graph $H \in \mathscr{G}(4p, p/2)$ such that $S = S_{01}(H)$ or there is a bipartite graph $B \in \mathscr{B}(4p, 3p/2)$

such that $S = S_{02}(B)$. In the first case it follows, as in the previous case, that H is trace-minimal. For the second case, $\mathrm{spec}(S_{01}(G)) = \mathrm{spec}(S_{01}(B'))$, by Eq. (42), and hence $\mathrm{spec}(A(B')) = \mathrm{spec}(A(G))$. Thus B' is trace-minimal.

7.7. $r \equiv -1 \pmod 4$

Let $r = 4d - 1$. As in the case $r \equiv 0 \pmod 4$, the minimum norm for a matrix in $\mathscr{M}(r)$ depends on how large d is in comparison to $p/2$. Let G be a graph in $\mathscr{G}(4p, 3p + d - 1)$ and let $S_{31}(G)$ be the remainder matrix defined in Eq. (12). Let B be a bipartite graph in $\mathscr{B}(4p, d)$ and let $S_{32}(B)$ be the remainder matrix defined in Eq. (13). Then

$$\|S_{31}(G)\|^2 = 4p(4d-1)^2 + 48p^2 - 32pd - 4p,$$
$$\|S_{32}(B)\|^2 = 4p(4d-1)^2 + 16p^2 + 32pd - 4p.$$

Lemma 30. *Let $r = 4d - 1$ and let $S \in \mathscr{M}(r)$. If $p/2 < d < p$, then*

$$\|S\|^2 \geqslant 4p(4d-1)^2 + 48p^2 - 32pd - 4p, \tag{43}$$

with equality if and only if there exists a graph G in $\mathscr{G}(4p, 3p + d - 1)$ such that $S = S_{31}(G)$.

Furthermore,

$$\det(4ptI_{4p} + S_{31}(G)) = \frac{4^{4p} t \,\mathrm{ch}_G(pt + d - 1)}{t - 3}. \tag{44}$$

If $0 \leqslant d < p/2$, then

$$\|S\|^2 \geqslant 4p(4d-1)^2 + 16p^2 + 32pd - 4p, \tag{45}$$

with equality if and only if there exists a bipartite graph B in $\mathscr{B}(4p, d)$ such that $S = S_{32}(B)$.

Furthermore,

$$\det(4ptI_{4p} + S_{32}(B)) = \frac{4^{4p}(p(t-1) + 2d)\mathrm{ch}_B(pt + d)}{pt + 2d}. \tag{46}$$

If $d = p/2$, then

$$\|S\|^2 \geqslant 4p(4d-1)^2 + 32p^2 - 36p,$$

with equality if and only if there exists a graph G in $\mathscr{G}(4p, 7p/2 - 1)$ such that $S = S_{31}(G)$, or there exist a bipartite graph B in $\mathscr{B}(4p, p/2)$ such that $S = S_{32}(B)$.

Proof. Let $S \in \mathscr{M}(r)$ and let $T = 4pI_{4p} - J_{4p} - S$. Then $T \in \mathscr{M}(4d')$, where $d' = p - d$. It is easy to verify that

$$\|S\|^2 = \|T\|^2 - 64p^3 - 16p^2 + 128p^2 d. \tag{47}$$

By Lemma 29 applied to T, we have

$$\|T\|^2 \geqslant 4p(4d')^2 + 64pd', \tag{48}$$

if $0 \leqslant d' < p/2$, and

$$\|T\|^2 \geqslant 4p(4d')^2 + 32p^2, \tag{49}$$

if $p/2 < d' < p$. Using Eq. (47), we find that inequality (43) is equivalent to inequality (48) and inequality (45) is equivalent to inequality (49).

To prove the cases for equality, first assume that $p/2 < d < p$ and that equality holds in inequality (43). Then equality holds in (48). Thus by Lemma 29, there exists a graph G' in $\mathscr{G}(4p, d')$ such that $T = 4d'I_{4p} - 4A(G')$. Let G be the complement of G'. Then $G \in \mathscr{G}(4p, 3p + d - 1)$ and $A(G') = J_{4p} - I_{4p} - A(G)$. Thus

$$\begin{aligned} S &= 4pI_{4p} - J_{4p} - T \\ &= 4(d-1)I_{4p} + 3J_{4p} - 4A(G) \\ &= S_{31}(G). \end{aligned}$$

We now prove Eq. (44). Since G is in $\mathscr{G}(4p, 3p + d - 1)$,

$$\mathrm{ch}_G(x) = (x - (3p + d - 1)) \prod (x - \lambda),$$

and

$$\mathrm{ch}_G(pt + d - 1) = p(t - 3) \prod (pt + d - 1 - \lambda),$$

where the products are taken over $\lambda \in \mathrm{spec}'(A(G))$. Thus the eigenvalues of $S_{31}(G) = 4(d-1)I_{4p} + 3J_{4p} - 4A(G)$ are $0, 4(d - 1 - \lambda)$, where $\lambda \in \mathrm{spec}'(A(G))$ so that

$$\begin{aligned} \det(4ptI_{4p} + S_{31}(G)) &= \det(4ptI_{4p} + 4(d-1)I_{4p} + 3J_{4p} - 4A(G)) \\ &= 4pt \prod (4pt + 4(d-1) - 4\lambda) \\ &= 4^{4p} pt \prod (pt + d - 1 - \lambda). \end{aligned}$$

It follows that

$$\det(4ptI_{4p} + S_{31}(G)) = \frac{4^{4p} t \,\mathrm{ch}_G(pt + d - 1)}{t - 3}.$$

Now assume that $0 \leqslant d < p/2$ and that equality holds in inequality (45). Then equality holds in inequality (49) as well. By Lemma 29, there exists a bipartite graph B' in $\mathscr{B}(4p, p + d')$ such that $T = S_{02}(B')$. Let

$$A(B') = \begin{bmatrix} 0 & N(B') \\ N(B')^{\mathrm{T}} & 0 \end{bmatrix}.$$

Then $N(B')$ is a (0, 1)-matrix and each row and column of $N(B')$ has exactly $d' + p = 2p - d$ ones. Thus

$$
\begin{aligned}
S &= 4pI_{4p} - J_{4p} - T \\
&= 4dI_{4p} + \begin{bmatrix} -J_{2p} & 4N(B') - 3J_{2p} \\ 4N(B')^{\mathrm{T}} - 3J_{2p} & -J_{2p} \end{bmatrix} \\
&= 4dI_{4p} + \begin{bmatrix} -J_{2p} & J_{2p} \\ J_{2p} & -J_{2p} \end{bmatrix} - 4\begin{bmatrix} 0 & A \\ A^{\mathrm{T}} & 0 \end{bmatrix},
\end{aligned}
$$

where $A = J_{2p} - N(B')$. Let B be the bipartite graph on $4p$ vertices with adjacency matrix

$$
A(B) = \begin{bmatrix} 0 & A \\ A^{\mathrm{T}} & 0 \end{bmatrix} = \begin{bmatrix} 0 & N(B) \\ N(B)^{\mathrm{T}} & 0 \end{bmatrix}.
$$

Then B is in $\mathscr{B}(4p, d)$ and $S = S_{32}(B)$.

We now prove Eq. (46). The eigenvalues of $A(B)$ are $\pm d, \pm\lambda$, where $\lambda \in \operatorname{sing}'(N(B))$. Thus

$$
\mathrm{ch}_B(x) = (x-d)(x+d)\prod(x-\lambda)(x+\lambda),
$$

and

$$
\mathrm{ch}_B(pt+d) = pt(pt+2d)\prod(pt+d-\lambda)(pt+d+\lambda),
$$

where the product runs over $\lambda \in \operatorname{sing}'(N(B))$. Next observe that 0 and $-4p$ are eigenvalues of the matrix

$$
\begin{bmatrix} -J_{2p} & J_{2p} \\ J_{2p} & -J_{2p} \end{bmatrix}
$$

with eigenvectors $[e_{2p}, \pm e_{2p}]^{\mathrm{T}}$. Thus $0, 8d - 4p, 4(d \pm \lambda)$ are eigenvalues of $S_{32}(B)$. Hence

$$
\begin{aligned}
&\det(4ptI_{4p} + S_{32}(B)) \\
&\quad = 4pt(4p(t-1) + 8d)\prod(4pt + 4d - 4\lambda)(4pt + 4d + 4\lambda) \\
&\quad = 4^{4p} pt(p(t-1) + 2d)\prod(pt + d - \lambda)(pt + d + \lambda) \\
&\quad = \frac{4^{4p}(p(t-1) + 2d)\mathrm{ch}_B(pt+d)}{pt + 2d}. \qquad \square
\end{aligned}
$$

7.8. *Proof of Lemma 18:* $r \equiv -1 \pmod 4$

This proof follows the same pattern as the proof of Lemma 19. The only difference is that if $p/2 < d < p$ and $G \in \mathscr{G}(4p, 3p + d - 1)$, then

$$
\operatorname{tr}(S_{31}(G)^i) = 4^i \sum_{j=0}^{i} \binom{i}{j} (-1)^j (d-1)^{i-j} [\operatorname{tr}(A(G)^j) - (3p + d - 1)^j],
$$

and if $0 \leqslant d < p/2$ and $B \in \mathscr{B}(4p, d)$, then

$$\operatorname{tr}(S_{32}(B)^i) = (8d - 4p)^i + 4^i \sum_{j=0}^{i} \binom{i}{j} d^{i-j} [\operatorname{tr}(A(B)^j) - d^j - (-d)^j].$$

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