Graph-Theoretic Techniques in D-Optimal Design Problems

Kashinath Chatterjee * Giri Narasimhan †

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Abstract

We solve several problems in D-Optimal Design theory using techniques from Graph theory and Combinatorics. The techniques involve relating the value of a determinant of a 0-1 matrix with the number of certain perfect matchings in a bipartite graph.

1 Introduction

Optimal saturated *main-effect* plans has been an area of considerable interest to Statistical theorists. Also, not much work has been done on D-optimal saturated *main-effect* plans (other than those given by orthogonal arrays) when the number of factors is three or more. Mukerjee, Chatterjee and Sen (1986) and Krafft (1988) showed that in the two factor case all such plans are equivalent with respect to D-optimality. Further results, including those related to other optimality criteria and extensions to mixed-effects models, were reported by Krafft (1988), Bagiatis (1990), Mandal, Shah and Sinha (1991), Bapat and Dey (1991) and Mukerjee, Shah and Sinha (1992). For the two factor case, Mukerjee and Sinha (1990) and Birkes and Dodge (1991) considered optimality results on almost saturated *main-effect* plans. Chatterjee and Mukerjee (1993) considered the case with three factors of which one factor is at two-level.

This paper considers the problem of finding D-optimal saturated *main-effect* plans involving three factors. The goal is to estimate the *main-effect* contrasts under the assumption that two-factor and higher order interactions are absent. A salient feature of this paper is the use of graph-theoretic techniques to solve problems in D-optimal design. Using graph-theoretic techniques, we give an alternative proof of the main theorem of Chatterjee and Mukerjee (1993), which provides a bound on the variance of the estimates of the *main-effect* contrasts and also provides a design attaining such a bound. We also give characterizations of designs that attain this bound. Graph-theoretic techniques were also useful in disproving a conjecture of Chatterjee (1994) related to generalizations of such designs. It is hoped that the present paper would serve as a starting point for using graph-theoretic techniques to further the study of general factorials and related combinatorial problems.

2 Statistical Preliminaries

We will mostly follow the notation of Chatterjee and Mukerjee (1993). Depending on the context, we will use the notation $|X|$ to refer to the determinant of a square matrix X, or to the cardinality of a set X.

*Department of Statistics, Asutosh College, 92, S. P. Mukherjee Road, Calcutta 700 026, India. This work was done while the author was visiting The University of Memphis;

†Department of Mathematical Sciences, The University of Memphis, Memphis TN 38152; *e-mail*: `Giri.Narasimhan@memphis.edu`; Supported in part by NSF Grant CCR-940-9752.

Consider a three-factor experiment in factors F_1, F_2 and F_3 at s_1, s_2 and s_3 levels respectively. Without loss of generality, $2 \leq s_2 \leq s_3$. To estimate the *main-effect* contrasts, the minimum number of runs required will be $n = 1 + (s_1 - 1) + (s_2 - 1) + (s_3 - 1) = s_1 + s_2 + s_3 - 2$. A plan in n runs allowing estimability of all *main-effect* contrasts under the absence of interaction effects will be called a *saturated main-effect plan.*

Each observation is associated with a level combination of the factors. Each of the $v = s_1 s_2 s_3$ level combinations will be denoted by a triplet $(i_1, i_2, i_3), i_j = 0, 1, \ldots, s_j - 1; j = 1, 2, 3$. An observation corresponding to the level combination (i_1, i_2, i_3) will be denoted by $y_{i_1 i_2 i_3}$. Let d denote a design, i.e., a fraction n of the v level combinations and let D denote all such designs. Let $\underline{1}_m$ be a column vector of m 1's and I_m be the identity matrix of order m. Let $\bigotimes$ denote the Kronecker product.

In a complete experiment (each level combination is experimented once), under the usual *fixed-effect linear model* and in the absence of interactions, we have

$$E(\underline{y}) = V\underline{\theta}, \quad Disp(\underline{y}) = \sigma^2 I, \tag{1}$$

where $\underline{y}$ is a vector with elements $y_{i_1 i_2 i_3}$ (lexicographically ordered) and, σ^2 is the unknown error variance, and $I = I_1 \bigotimes I_2 \bigotimes I_3$. Also,

$$\theta = (\mu, \underline{\beta}_1', \underline{\beta}_2', \underline{\beta}_3')'$$

where μ is the (unknown) general mean, and for $j = 1, 2, 3$, the $(s_j - 1)$ elements of $\underline{\beta}_j$ are unknown parameters representing a full set of mutually orthogonal contrasts belonging to the *main-effect* F_j (cf., Mukerjee and Sinha (1990)). Let

$$X = [\underline{\varepsilon}, X_1, X_2, X_3] \tag{2}$$

where

$$\begin{aligned}
\underline{\varepsilon} &= \underline{1}_{s_1} \bigotimes \underline{1}_{s_2} \bigotimes \underline{1}_{s_3}, \\
X_1 &= I_{s_1} \bigotimes \underline{1}_{s_2} \bigotimes \underline{1}_{s_3}, \\
X_2 &= \underline{1}_{s_1} \bigotimes I_{s_2} \bigotimes \underline{1}_{s_3}, and \\
X_3 &= \underline{1}_{s_1} \bigotimes \underline{1}_{s_2} \bigotimes I_{s_3}
\end{aligned}$$

Then following Chatterjee and Mukerjee(1993), one may obtain

$$V = UH$$

where U is a submatrix of X of order $v \times n$ given by

$$U = [X_1^*, \ X_2^*, \ X_3]$$

and $X_1^*(X_2^*)$ is obtained from $X_1(X_2, respectively)$ by deleting the last column of the latter. Also H is a non- singular matrix of order n. The rows of U, like those of V, correspond to the lexicographically ordered level combinations.

Our goal is to estimate complete sets of contrasts belonging to the *main-effects* of factors F_1, F_2, and F_3. For any plan $d \in D$, the design matrix is given by $V_d = U_d H$, where U_d is a square submatrix of U of order n and the rows of U_d are determined by the level combinations included in d. Since H is non-singular, it is clear that a plan $d_0 \in D$ is *D-Optimal* for the estimation of $\underline{\theta}$ iff

$$|U_{d_0}' U_{d_0}| = \max_{d \in D} \{|U_d' U_d|\}.$$

Equivalently, a plan $d_0 \in D$ is *D-Optimal* iff

$$\mathrm{abs}(|U'_{d_0}|) = \max_{d \in D}\{\mathrm{abs}(|U'_d|)\}$$

Note that for any plan $d \in D$, the matrix U'_d is a 0-1 matrix satisfying property $\mathcal{P}_i$ (for $i = s_1 - 1$), where property $\mathcal{P}_i$ is defined as follows:

Property $\mathcal{P}_i$: A 0-1 square matrix satisfies property $\mathcal{P}_i$, if its rows can be partitioned into 3 sets S_1, S_2, S_3, such that $|S_1| = i$ and any column has at most one 1 in each of S_1, S_2, S_3.

We reduce the problem of finding the maximum determinant of a 0-1 matrix satisfying property $\mathcal{P}_i$ to that of finding the number of certain kinds of perfect matchings in restricted bipartite graphs. We first consider the case when $i = 1$. These results are presented in section 4. We then consider the case $i = 2$, the results of which are presented in section 5.

3 Graph-Theoretic Notation and Preliminaries

In this section, we first introduce notation from graph theory and concepts that are necessary to describe the techniques used.

Let $G(A, B, E)$ be a *bipartite graph* with the vertex set partitioned into sets A and B each of size n, and edge set E. Let X be the *adjacency matrix* of G, which is a 0-1 square matrix of order n with rows corresponding to the elements of A and columns corresponding to the elements of B. By definition, $X[i, j]$ equals 1 if $i \in A, j \in B$ and $(i, j) \in E$; it equals 0 otherwise.

A *matching* in a bipartite graph is a set of edges that do not share any vertices in common. A *perfect matching* in a bipartite graph, as considered above, is a matching that is incident on every vertex of the graph. From this point onwards, whenever we refer to matchings we will mean perfect matchings, although some of the statements may be true about general matchings as well. Every perfect matching M can be associated with a permutation σ_M such that edge $(i, \sigma_M(i)) \in M$. Conversely, if a permutation σ_M is such that $(i, \sigma_M(i)) \in E$, then it can be associated with a perfect matching M consisting of the edges $(i, \sigma_M(i))$; such a permutation will be called a *non-void permutation.*

We next discuss some notations and properties related to permutations. In a permutation σ, if $i < j$ and $\sigma(i) > \sigma(j)$, the pair $(\sigma(i), \sigma(j))$ is called an *inversion* of the permutation. A permutation is an *even permutation* if the number of inversions of the permutation is even; otherwise, it is an *odd permutation.* One well-known property of permutations (cf., Knuth, (1973), section 5.1) is that if two elements are exchanged in an even (odd) permutation, it becomes an odd (even, resp.) permutation. For a graph, a perfect matching is called an *even matching*, if it is associated with an even permutation; otherwise it is an *odd matching.*

Following Mulmuley, Vazirani, and Vazirani (1987), for each permutation σ on $\{1, 2, \ldots, n\}$, define

$$value(\sigma) = \prod_{i=1}^{n} X[i, \sigma(i)]$$

where X is the adjacency matrix of the bipartite graph. It is clear that $value(\sigma)$ equals 1 iff σ is a non-void permutation. By Cramer's definition, the determinant of X is given by

$$|X| = \sum_{\sigma} sign(\sigma) value(\sigma),$$

where $sign(\sigma)$ is $+1$ if σ is an even permutation, and -1 otherwise. Thus, a perfect matching corresponds to a non-zero term in determinant expansion of the adjacency matrix, although it may contribute a $+1$ or a -1. Thus the determinant of an adjacency matrix is the difference between the number of even perfect matchings and the number of odd perfect matchings of a bipartite graph.

We denote the *symmetric difference* operator on two sets by the symbol Δ. It is known that (cf., Lovasz and Plummer (1986)) given two perfect matchings M and M', $M \Delta M'$ is a collection of cycles of even length. We prove the following lemma about perfect matchings in a bipartite graph.

Lemma 1 *Given two perfect matchings M and M' such that $M \Delta M'$ is exactly equal to a single cycle C of length $4m$ (for some integer m), M is an even matching iff M' is an odd matching. Also, given two perfect matchings M and M' such that $M \Delta M'$ is exactly equal to a single cycle C of length $4m+2$ (for some integer m), M is an even matching iff M' is an even matching.*

Proof. Assume that M is an even matching. This implies that it can be represented by an even permutation π. Let M' be represented by the permutation π'. Recall that any permutation can be written down in two-line form as follows:

$$\begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ x_1 & x_2 & x_3 & \cdots & x_n \end{pmatrix}$$

Let cycle C consists of the sequence of vertices $y_1, z_1, y_2, z_2, \ldots, y_k, z_k, y_1$. Let C be partitioned into two edge sets C_1 and C_2 so that neither C_1 nor C_2 contains adjacent edges. Let $C_1 = \{(y_i, z_i), i = 1, \ldots, k\}$ and let C_2 contain the rest of the edges from C. Let $C_1 \subseteq M$ and $C_2 \subseteq M'$. Thus edges in C_1 correspond to a subsequence of the permutation π, which we will refer to as π_1. Similarly, C_2 corresponds to a subsequence of the permutation π', which we will refer to as π_2. The permutations π and π' are identical except that π contains π_1, which is replaced by π_2 in π'. If C is of length $2k$ then π_1 and π_2 are of length k. Thus if C is of length $4m$ for some m, then π_1 and π_2 are of even length, otherwise they are of odd length. Thus using the two-line notation π_1 can be written down in the form

$$\begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_k \\ z_1 & z_2 & z_3 & \cdots & z_k \end{pmatrix}$$

It is easy to see that using the above representation for π_1, we can write down π_2 in the form

$$\begin{pmatrix} y_1 & y_2 & y_3 & \cdots & y_k \\ z_k & z_1 & z_2 & \cdots & z_{k-1} \end{pmatrix}$$

Permutation π_2 can be obtained from π_1 by doing exactly $k-1$ exchanges. Similarly, permutation π' can be obtained from π by doing exactly $k-1$ exchanges. Each exchange switches the parity of the permutation (from even to odd, or from odd to even). It is thus easy to see that if $k = 2m$, then matching M is even iff M' is odd. Also, if $k = 2m+1$, then matching M is even iff M' is even. $\Box$

4 0-1 Matrices that Satisfy Property $\mathcal{P}_1$

Let X^* be a 0-1 matrix of order n that satisfies property $\mathcal{P}_1$ and that has the maximum determinant value. Let $G^*(A, B, E)$ be the bipartite graph with adjacency matrix X^*. Let the rows of X^* be partitioned into 3 sets S_1, S_2, S_3, such that $|S_1| = 1$ and any column has at most one 1 in each of

S_1, S_2, S_3. Without loss of generality, we will assume that $|S_2| \leq |S_3|$. Let the set of vertices of A associated with rows S_2 and S_3 be A_2 and A_3 respectively. Let c be the vertex of G^* associated with the singleton row of S_1 and let $F = \{e_1, e_2, \ldots, e_k\}$ be the set of edges incident on vertex c. Let N be the set of perfect matchings of G^* that contribute a non-zero value to the determinant of X^*. Any perfect matching in N includes exactly one edge from F. Let N_i be the set of perfect matchings in N that include edge e_i. Thus $N = \cup_{i=1}^{k} N_i$. As discussed earlier, the matchings in N_i will contribute either $+1$ or -1 towards the value of the determinant. Let m_i be the net contribution of the matchings in N_i towards the value of the determinant of X^*. We prove the following theorem:

Theorem 1 *The absolute value of the determinant of X^* equals $|S_2| + 1$.*

We need a few lemmas for proving Theorem 1.

Lemma 2 *Any cycle C that does not pass through c is of length $4m$ for some integer m.*

Proof. Follows because every column vertex can be adjacent to at most one vertex from each of A_2 and A_3. $\square$

Note that the converse of Lemma 2 need not be true.

Lemma 3 *Assume that there exists a cycle C that does not pass through c. Let C be partitioned into two edge sets C_1 and C_2 so that neither C_1 nor C_2 contains adjacent edges. Any perfect matching M must either include an edge from c to a vertex of C, or it must include all of C_1, or it must include all of C_2.*

Proof. Assume that M does not include an edge from c to a (column) vertex of C. For every column vertex x on the cycle C, if we ignore the possible edge it might have connecting it to vertex c, it must have only two more edges incident on it and both these edges must be on cycle C. Thus M must include one of these two edges and consequently must have every edge of C_1 or every edge of C_2. $\square$

Lemma 3 further implies that if M contains all the edges of C_1, then there exists a unique matching M' (containing all edges of C_2) such that $M \Delta M'$ is exactly C, which, by Lemma 2, is of length $4m$. By Lemma 1,it follows that M must be an odd matching iff M' is an even matching.

Lemma 4 $|m_i| \leq 1$

Proof. Assume that $|N_i| \geq 2$. Given any two perfect matchings in N_i, their symmetric difference must consist of one or more cycles that do not pass through either endpoint of edge e_i (i.e., if $e_i = (c, b_i)$, then these cycles avoid both c and b_i.). Let C be a fixed cycle that does not pass through vertex c. Clearly, C is of length $4m$, for some integer m. Let C be partitioned into two edge sets C_1 and C_2 so that neither C_1 nor C_2 contains adjacent edges. Thus, by Lemma 3, every matching $M \in N_i$ must include all edges from C_1 or all edges from C_2; note that since M contain edge e_i, it does not contain any edge from c to C. For any matching $M \in N_i$, consider the (unique) matching $M' \in N_i$ such that $M \Delta M' = C$. By Lemma 2, M is an even matching iff M' is odd. This implies that the contribution of every matching in N_i towards the determinant is canceled out by another uniquely specified matching. Thus $m_i = 0$. It is also clear that if $|N_i| = 1$, then $m_i = \pm 1$. Hence the result. $\square$

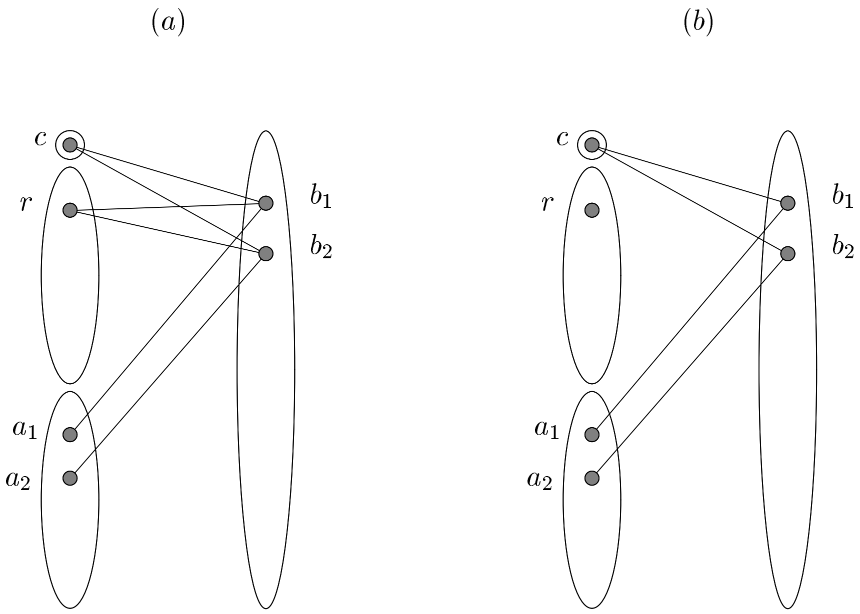

Figure 1: Figures for Lemma 5

Since $|m_i| \leq 1$, it is clear that $\text{abs}(|X^*|) \leq k$, where $k = |F|$ is the degree of vertex c. Let

$$F' = \{e_i \mid e_i \in F; |N_i| = 1\}.$$

Let M_i be the unique perfect matching that contains edge $e_i \in F'$. Let

$$\mathcal{M}' = \{M_i \mid e_i \in F'\}$$

Let $\mathcal{M}''$ be the largest subset of $\mathcal{M}'$ such that every matching of $\mathcal{M}''$ has the same parity. Finally, let F'' be the subset of edges from F' that are contained in some matching in $\mathcal{M}''$. Note that $\text{abs}(|X^*|) = \text{abs}(|\mathcal{M}''| - |\mathcal{M}'|)$. Thus $|\mathcal{M}''| = |F''|$ is an upper bound on the absolute value of $|X^*|$.

Lemma 5 $|F''| \leq |S_2| + 1$

Proof. Let $|F''| \geq |S_2| + 2$. Let B'' be the set of column vertices that are incident on the edges in F''. Clearly $|B''| \geq |S_2| + 2$. Note that each vertex in B'' is adjacent to at most one vertex from A_2, the vertex set corresponding to rows in S_2. A simple application of the *pigeon hole principle* shows that some pair of vertices in B'' must either be adjacent to the same vertex in A_2 or adjacent to no vertex in A_2. These two situations are illustrated in Figure 1. We show below that under these conditions, there must be two perfect matchings from $\mathcal{M}''$ that have different parity contradicting the definition of F''.

Consider the situation of Figure 1. Let b_1 and b_2 be two vertices from B'' that are connected to c by edges e_1 and e_2. Also assume that b_1 and b_2 are both adjacent to a common vertex $r \in A_2$. Let M_1 and M_2 be the unique perfect matchings from $\mathcal{M}''$ that include e_1 and e_2 respectively. If edge $(r, b_2) \in M_1$, then clearly, (r, b_1) must be in M_2 and the two matchings are consequently of different parity (since their symmetric difference is a single cycle of length 4), which contradicts the definition of $\mathcal{M}''$. Hence, in order to cover vertex b_2, matching M_1 must include an edge (b_2, a_2), where $a_2 \in A_3$. By a similar argument, in order to cover vertex b_1, matching M_2 must include

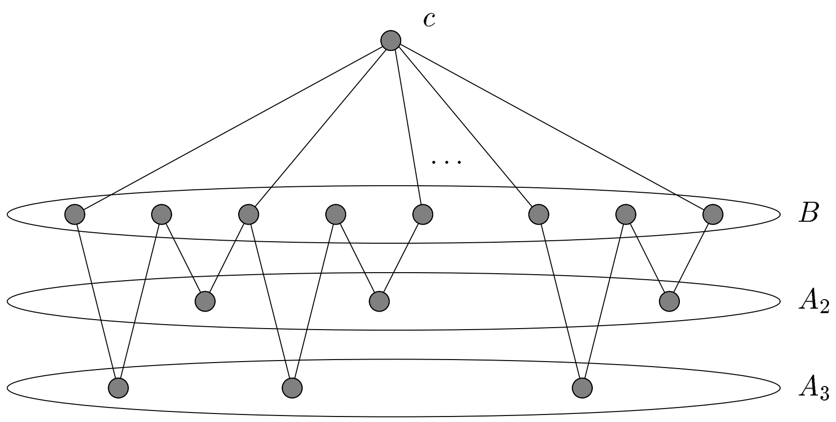

Figure 2: Figures for Lemma 6

an edge (b_1, a_1), where $a_1 \in A_3$. Consider the cycle C in $M_1 \Delta M_2$ that includes vertex c; clearly, such a cycle must exist. By the conditions described above, C must include (besides c) vertices $b_1, b_2 \in B$, and $a_1, a_2 \in A_3$. But then the cycle can never be completed since no column vertex can be adjacent to two vertices in A_2 or in A_3. Hence the situation in Figure 1(a) cannot take place. A similar argument rules out the possibility of the situation of Figure 1(b). Hence the result. □

Lemma 6 $\text{abs}(|X^*|) \geq |S_2| + 1$

Proof. Following the proof of Chatterjee and Mukerjee (1993), we consider the graph G shown in Figure 2. $G(A, B, E)$ is a bipartite graph, where $A = A_2 \cup A_3 \cup \{c\}$. Note that for any positive integer p, B has $2p + 1$ vertices, while A_1 and A_2 have p vertices each. The edges are as shown in the figure. It is straightforward to verify that the adjacency matrix of G has $|S_2| + 1$ as the absolute value of its determinant. Thus $\text{abs}(|X^*|) \geq |S_2| + 1$. □

Lemma 5 and Lemma 6 together prove Theorem 1. We have thus provided a simpler and more transparent proof of the findings in Chatterjee and Mukerjee (1993).

5 0-1 Matrices that Satisfy Property $\mathcal{P}_2$

Let X^* be a 0-1 matrix of order n that satisfies property $\mathcal{P}_2$ and that has the maximum determinant value. Chatterjee (1994) conjectured that the level combinations described below gives a D-optimal design for this case, namely, the $3 \times s_2 \times s_3$ case. Their conjecture considered the two cases when s_2 is odd and when s_2 is even as described below.

Conjecture 1 [Chatterjee (1994)]
Case 1: *For $s_2 = 2k + 1$, the level combinations of a D-optimal design are*

$$(0, 0, s_2 - 1), (0, i, i - 1)(1 \leq i \leq k - 1), (0, s_2 - 1, k - 1), (1, k, s_2 - 1), (1, i, i - 1)(k + 1 \leq i \leq s_2 - 1), (2, i, i)(0 \leq i \leq s_2 - 2), (2, s_2 - 1, j)(s_2 - 1 \leq j \leq s_3 - 1).$$

Case 2. *For $s_2 = 2k + 2$, the level combinations of a D-optimal design are either*

(a) $(0, 0, s_2 - 1), (0, i, i - 1)(1 \leq i \leq k - 1), (0, s_2 - 1, k - 1), (1, k, s_2 - 1), (1, i, i - 1)(k + 1 \leq i \leq s_2 - 1), (2, i, i)(0 \leq i \leq s_2 - 2), (2, s_2 - 1, j)(s_2 - 1 \leq j \leq s_3 - 1)$, *or*

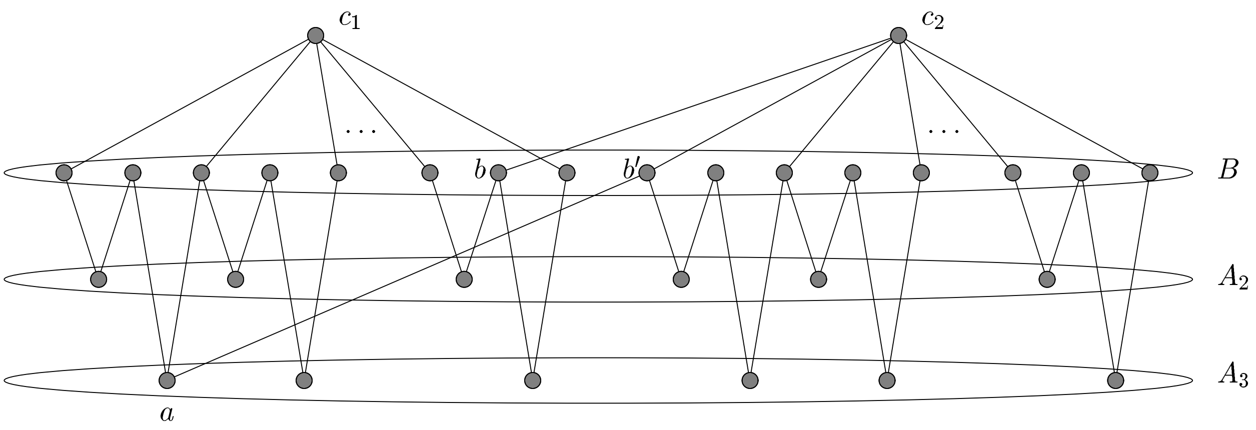

Figure 3: Graph Disproving Conjecture 1

(b) $(0, 0, s_2 - 1), (0, i, i - 1)(1 \leq i \leq k), (0, s_2 - 1, k), (1, k + 1, s_2 - 1), (1, i, i - 1)(k + 2 \leq i \leq s_2 - 1), (2, i, i)(0 \leq i \leq s_2 - 2), (2, s_2 - 1, j)(s_2 - 1 \leq j \leq s_3 - 1)$.

Furthermore, if U_d is the submatrix of U corresponding to any of the above design, then

$$\mathrm{abs}(|U_d|) = \begin{cases} (k+1)^2, & \text{if } s_2 = 2k+1, \\ k(k+1), & \text{if } s_2 = 2k \end{cases}$$

Note that the total number of level combinations in all the cases is $1 + s_2 + s_3$, which is same as the number of level combinations for a *saturated main-effect plan*.

In Figure 3, we present a bipartite graph $G(A, B, E)$ that disproves the above conjecture. Note that $A = A_2 \cup A_3 \cup \{c_1, c_2\}$. Also, $|A_2| = |A_3| = 2k$ and $|B| = 2k + 2$, for some integer k. The edges of the graph G are as shown in the figure. The graph G consists of two copies of the graph from Figure 2 with two extra edges, namely, (c_2, b) and (b', a). We claim that the graph G has an adjacency matrix X^* such that

$$\mathrm{abs}(|X^*|) = (k+1)^2 + 1.$$

We now argue that the claim is true. Let $B_1 \subset B$ be the set of vertices adjacent to vertex c_1; let B_2 be the set of vertices that are adjacent to c_2 and that are in $B \backslash \{b\}$. It is easy to see that for every choice of an edge from c_1 to B_1, and an edge from c_2 to B_2, there is a unique perfect matching that contributes a non-zero value to the determinant. Since there are $(k+1)^2$ choices of these edges, there are $(k+1)^2$ different perfect matchings arising from these choices that contribute to the determinant value. It is easy to see that all of them have the same parity. Therefore, the sum of their contribution to the absolute value of the determinant is $(k+1)^2$. Now consider any perfect matching M that includes edge (c_2, b). It is easy to see that M must include the edge (b', a). However, there is a unique perfect matching M that includes both the edges (c_2, b) and (b', a). Furthermore, they are of the same parity as the other $(k+1)^2$ perfect matchings mentioned above. Since no other perfect matchings could possibly exist, the claim is proved, and Conjecture 1 is disproved.

The design that corresponds to the example in Figure 3 is for the case when $s_2 = 2k + 1$; the design in this case is: $(0, 0, s_2 - 1), (0, i, i - 1)(1 \leq i \leq k - 1), (0, s_2 - 1, k - 1), (1, k, 0), (1, i, i - 1)(k + 1 \leq i \leq s_2 - 1), (1, 1, 1), (2, 0, 0), (2, i, i)(2 \leq i \leq s_2 - 2), (2, s_2 - 1, j)(s_2 - 1 \leq j \leq s_3 - 1)$.

6 Conclusion

Graph-theoretic and combinatorial techniques have been found useful in solving problems in D-optimal designs.

In order to solve the more general D-optimal design problem, we need to find the maximum determinant of 0-1 matrices that satisfy property $\mathcal{P}_k$ for arbitrary values of k. This problem remains open.

For the case of 0-1 matrices satisfying $\mathcal{P}_2$, even though we have disproved conjecture 1, the problem of finding a D-optimal design remains open. Furthermore, we conjecture that the design we presented as a counterexample to conjecture 1 does, indeed, represent the D-optimal design.

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