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Two-level search design for main-effect plus two plan

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Abstract. One important class of screening designs is the search design first proposed by Srivastava (1975). A new class of two-level factorial search designs which are capable of estimating all main-effect plus two interactions is provided. We first give a necessary and sufficient condition for the main-effect plus two plan and then show that the proposed search design always satisfies such a condition.

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Key words: Two-level factorial design; level combination of factors; two-factor interaction; three-factor interaction

1. Introduction

Ever since the pioneering work of Srivastava (1975), a substantial amount of research has been done in the field of search designs. Recent research trends in this area exhibit a considerable interest in the development of search designs which, in addition to ensuring estimability of the parameters known to be present, are capable of searching and estimating K possibly present parameters. In this connection, mention may be made to Shirakura (1991), Srivastava and Arora (1987), Srivastava (1992), Chatterjee and Mukerjee (1986), and Mukerjee and Chatterjee (1994).

Much work has been done for constructing search designs for $K = 1$. See, for example, Ghosh (1980) and Gupta (1991). In this paper, we suggest a new

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class of search designs for two-level factorials which are capable of estimating the grand mean and all the main effects and allow the searching and estimating of at least two interactions among all the two- or three-factor interactions, assuming that four- and higher-order interactions are absent.

Consider the linear model below: Let $\mathbf{Y}$ be an $N \times 1$ vector of observations with

$$E(\mathbf{Y}) = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2, \quad \text{Disp}(\mathbf{Y}) = \sigma^2\mathbf{I}_N \tag{1}$$

where $\mathbf{X}_1, \mathbf{X}_2$ are the design matrices of order $N \times n_1$ and $N \times n_2$, respectively; $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2$ are the vectors of parameters of order $n_1 \times 1$ and $n_2 \times 1$, respectively; and $\mathbf{I}_N$ is an identity matrix of order N. Furthermore, only K elements of $\boldsymbol{\beta}_2$ are assumed to be non-zero, where K is relatively small compared to n_2. Here, the objective is to provide a design which will estimate the grand mean and all the main-effects ($\boldsymbol{\beta}_1$) and permit the detection and estimation of the non-zero elements of $\boldsymbol{\beta}_2$. In this paper, we will consider the "noiseless" case with $\sigma^2 = 0$, as in Srivastava (1975). The main theorem in this field is provided by Srivastava (1975), as stated in Theorem 1.

Theorem 1. *A necessary and sufficient condition that the above problem will be completely solved is that for any submatrix $\mathbf{X}_2^*$ of $\mathbf{X}_2$ of order $N \times 2K$, we have*

$$\text{rank}[\mathbf{X}_1, \mathbf{X}_2^*] = n_1 + 2K.$$

2. Notations and preliminaries

Consider a factorial experiment involving m factors $F_1, F_2, \ldots, F_m$ each at two levels. Let the levels of the factors be coded as $0, 1$ and a typical level combination of these factors be denoted by $(f_1, f_2, \ldots, f_m)$, $f_i = \{0, 1\}$, for $1 \le i \le m$. For any positive integer n, let $\mathbf{I}_n$ denote the identity matrix of order n, and let $\mathbf{0}_n$ and $\mathbf{1}_n$ denote the n column vectors with all elements 0 and 1, respectively. Let $\mathbf{1}_{n\times m}$ and $\mathbf{O}_{n\times m}$ denote the matrices of order $n \times m$ with entry values 1 and 0, respectively. For the simplicity of presentation, we may drop the subscripts hereafter.

Suppose prior information is available regarding the absence of all interactions involving four or more factors and it is known that among the two- and three-factor interactions at most two are non-negligible, although these interactions are not known a priori. Then, under model (1) by taking $\boldsymbol{\beta}_1$ as the grand mean and main effects and $\boldsymbol{\beta}_2$ as the two- and three-factor interactions, it is easy to see that if one observation is made for each of the $v = (2^m)$ level combinations of $F_1, F_2, \ldots, F_m$, the resulting design matrix will be of the form

$$\mathbf{X} = [\mathbf{1}_v, \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m, \mathbf{u}_{12}, \ldots, \mathbf{u}_{m-1,m}, \mathbf{u}_{123}, \ldots, \mathbf{u}_{m-2,m-1,m}], \tag{2}$$

where $\mathbf{u}_i$ is a vector of ± 1 for $1 \le i \le m$ and

$$\mathbf{u}_{ij} = \mathbf{u}_i * \mathbf{u}_j, \quad 1 \le i < j \le m;$$

$$\mathbf{u}_{ijk} = \mathbf{u}_i * \mathbf{u}_j * \mathbf{u}_k, \quad 1 \le i < j < k \le m,$$

and '$*$' denotes the Hadamard product. The Hadamard product of two vectors $\mathbf{u} = (u_1, u_2, \ldots, u_m)'$ and $\mathbf{v} = (v_1, v_2, \ldots, v_m)'$ is defined as $\mathbf{u} * \mathbf{v} = (u_1v_1, u_2v_2, \ldots, u_mv_m)'$. Observe that in the above, $\mathbf{1}_v$ corresponds to the grand mean, $\mathbf{u}_i$ corresponds to the main effect F_i $(1 \le i \le m)$, $\mathbf{u}_{ij}$ corresponds to the two-factor interaction F_iF_j $(1 \le i < j \le m)$, and finally, $\mathbf{u}_{ijk}$ corresponds to the three-factor interaction $F_iF_jF_k$ $(1 \le i < j < k \le m)$. It follows that

$$\mathbf{X}_1 = [\mathbf{1}_v, \mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m] = [\mathbf{1}_v, \mathbf{U}_1] \quad \text{and}$$

$$\mathbf{X}_2 = [\mathbf{u}_{12}, \ldots, \mathbf{u}_{m-1,m}, \mathbf{u}_{123}, \ldots, \mathbf{u}_{m-2,m-1,m}] = [\mathbf{U}_2, \mathbf{U}_3].$$

Let $\mathbf{Q}$ be a subset of N level combinations of $F_1, F_2, \ldots, F_m$ with the corresponding submatrices of $\mathbf{X}_1$ and $\mathbf{X}_2$ as

$$\mathbf{X}_1^* = [\mathbf{1}_N, \mathbf{u}_1^*, \mathbf{u}_2^*, \ldots, \mathbf{u}_m^*] = [\mathbf{1}_N, \mathbf{U}_1^*] \quad \text{and}$$

$$\mathbf{X}_2^* = [\mathbf{u}_{12}^*, \ldots, \mathbf{u}_{m-1,m}^*, \mathbf{u}_{123}^*, \ldots, \mathbf{u}_{m-2,m-1,m}^*] = [\mathbf{U}_2^*, \mathbf{U}_3^*].$$

respectively. Clearly, a minimum requirement for choosing N runs is that $\text{rank}(\mathbf{X}_1^*) = m + 1$. Then, analogous to Theorem 1, we have the following theorem. In the next section, we will provide a new class of the search designs that satisfies such a requirement.

Theorem 2. *A necessary and sufficient condition that* $\mathbf{Q}$ *represents a search design for estimating all main-effects and searching and estimating the possibly present interactions of at most two of the two- and three-factor interactions if the following holds: for any submatrix* $\mathbf{X}_2^{**}$ *of* $\mathbf{X}_2^*$ *of order* $N \times 4$, *we have a full-rank matrix* $[\mathbf{X}_1^*, \mathbf{X}_2^{**}]$. *That is,*

$$\text{rank}[\mathbf{X}_1^*, \mathbf{X}_2^{**}] = m + 5.$$

3. A new class of two-level search designs

Define the following $m \times N$ matrix

$$\mathbf{Q} = [\mathbf{0}_m, \mathbf{I}_m, \mathbf{R}_m], \tag{3}$$

where $\mathbf{R}_m$ is a $m \times \binom{m}{2}$ matrix with its column vector $\mathbf{r}_{ij} = \mathbf{1}_m - \mathbf{e}_i - \mathbf{e}_j$, where $\mathbf{e}_i, \mathbf{e}_j$ are the i-th and j-th unit vectors. The matrix $\mathbf{R}_m$ consists of columns with 0 in the i, j-th position and 1 in the other positions for $1 \le i < j \le m$. Consequently, the number of columns in $\mathbf{Q}$ is $N = 1 + m + \binom{m}{2}$.

Each column of $\mathbf{Q}$ corresponds to a level combination of m factors $F_1, F_2, \ldots, F_m$. Therefore, the design corresponding to the matrix $\mathbf{Q}$ is

1. For the first run, set all m factors to low.
2. For the next m runs, for $i = 1, 2, \ldots, m$, set factor F_i to high and set other factors to low.
3. For the next $\binom{m}{2}$ runs, for $1 \le i < j \le m$, set factors F_i and F_j to low and other factors to high.

We next present some properties of such a $\mathbf{Q}$ matrix and then prove that a search design based on $\mathbf{Q}$ will always satisfy Theorem 2.

For example, when $m = 8$, $\mathbf{R}_8$ is the 8×28 matrix

$$\begin{matrix}
0&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
0&1&1&1&1&1&1&0&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1&1&1&1&1&1\\
1&0&1&1&1&1&1&0&1&1&1&1&1&0&0&0&0&0&1&1&1&1&1&1&1&1&1&1\\
1&1&0&1&1&1&1&1&0&1&1&1&1&0&1&1&1&1&0&0&0&0&1&1&1&1&1&1\\
1&1&1&0&1&1&1&1&1&0&1&1&1&1&0&1&1&1&0&1&1&1&0&0&0&1&1&1\\
1&1&1&1&0&1&1&1&1&1&0&1&1&1&1&0&1&1&1&0&1&1&0&1&1&0&0&1\\
1&1&1&1&1&0&1&1&1&1&1&0&1&1&1&1&0&1&1&1&0&1&1&0&1&0&1&0\\
1&1&1&1&1&1&0&1&1&1&1&1&0&1&1&1&1&0&1&1&1&0&1&1&0&1&0&0
\end{matrix}$$

and therefore $\mathbf{Q} = [\mathbf{0}_8, \mathbf{I}_8, \mathbf{R}_8]$ and $N = 1 + 8 + \binom{8}{2} = 37$. The design matrix in (3) can be written as

$$\mathbf{X}^* = [\mathbf{1}_N, \mathbf{U}_1^*, \mathbf{U}_2^*, \mathbf{U}_3^*], \tag{4}$$

where

- $\mathbf{U}_1^* = [\mathbf{u}_1^*, \mathbf{u}_2^*, \ldots, \mathbf{u}_m^*]$, where $\mathbf{u}_i^* = 2\mathbf{q}_i - \mathbf{1}$ and $\mathbf{q}_i$ is a column vector of $\mathbf{Q}'$.
- $\mathbf{U}_2^* = [\mathbf{u}_{12}^*, \ldots, \mathbf{u}_{m-1,m}^*]$, where $\mathbf{u}_{ij}^* = \mathbf{u}_i^* * \mathbf{u}_j^*$.
- $\mathbf{U}_3^* = [\mathbf{u}_{123}^*, \ldots, \mathbf{u}_{m-2,m-1,m}^*]$, where $\mathbf{u}_{ijk}^* = \mathbf{u}_i^* * \mathbf{u}_j^* * \mathbf{u}_k^*$.

Since $\mathbf{u}_i^* = 2\mathbf{q}_i - \mathbf{1}$, we have $\mathbf{q}_i = (\mathbf{u}_i^* + \mathbf{1})/2$. That is, the column vectors in $\mathbf{U}_1^*$ can be transformed into column vectors in

$$\mathbf{Q}' = \begin{bmatrix} \mathbf{0}_m' \\ \mathbf{I}_m \\ \mathbf{R}_m' \end{bmatrix} = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_m].$$

Note also that $\mathbf{u}_{ij}^* = (2\mathbf{q}_i - \mathbf{1}) * (2\mathbf{q}_j - \mathbf{1}) = 4\mathbf{q}_i * \mathbf{q}_j - 2(\mathbf{q}_i + \mathbf{q}_j) + \mathbf{1}$. Therefore, $(\mathbf{u}_{ij}^* + 2(\mathbf{q}_i + \mathbf{q}_j) - \mathbf{1})/4 = \mathbf{q}_i * \mathbf{q}_j$. The entry value of $\mathbf{q}_i * \mathbf{q}_j$ is 1 only when the corresponding entries of both $\mathbf{q}_i$ and $\mathbf{q}_j$ are 1. The column vectors in $\mathbf{U}_2^*$ can be transformed into column vectors in

$$\begin{bmatrix} \mathbf{0}'_{\binom{m}{2}} \\ \mathbf{O}_{m\times\binom{m}{2}} \\ \mathbf{V}_1 \end{bmatrix} = [\mathbf{q}_1 * \mathbf{q}_2, \ldots, \mathbf{q}_{m-1} * \mathbf{q}_m],$$

where $\mathbf{V}_1 = [\mathbf{v}_{12}, \ldots, \mathbf{v}_{m-1,m}]$ is a $\binom{m}{2} \times \binom{m}{2}$ matrix and the value of the entry of $\mathbf{v}_{ij}$ $(1 \le i < j \le m)$ will be 1 when both i-th and j-th factors are set to be 1. Otherwise, the value will be 0. Note that there are exactly $\binom{m-2}{2}$ entries of each $\mathbf{v}_{ij}$ vector that are 1 with the remaining entries equal to 0.

Similarly, it is straightforward to see that

$$-(\mathbf{u}_{ijk}^* - 2(\mathbf{q}_i + \mathbf{q}_j) + \mathbf{1})/4 = -2\mathbf{q}_i * \mathbf{q}_j * \mathbf{q}_k + (\mathbf{q}_i * \mathbf{q}_j + \mathbf{q}_i * \mathbf{q}_k + \mathbf{q}_j * \mathbf{q}_k) \equiv \mathbf{p}_{ijk}.$$

We can see that $\mathbf{p}_{ijk}$ value is 1 for the cases of $(\mathbf{q}_i, \mathbf{q}_j, \mathbf{q}_k) = (0,1,1), (1,0,1), (1,1,0), (1,1,1)$ and is 0 otherwise. In other words, the entry value of $\mathbf{p}_{ijk}$ is 1 only when two or more of the corresponding entries of $\mathbf{q}_i$, $\mathbf{q}_j$ and $\mathbf{q}_k$ have value 1. Therefore, within this vector all the entries corresponding to $\mathbf{0}'_m$ and $\mathbf{I}_m$ in $\mathbf{Q}' = [\mathbf{0}_m, \mathbf{I}_m, \mathbf{R}_m]'$ will be 0. Thus, the column vectors in $\mathbf{U}_3^*$ can be transformed into column vectors in

$$\begin{bmatrix} \mathbf{0}'_{\binom{m}{3}} \\ \mathbf{O}_{m\times\binom{m}{3}} \\ \mathbf{V}_2 \end{bmatrix},$$

where $\mathbf{V}_2 = [\mathbf{w}_{123}, \ldots, \mathbf{w}_{m-2,m-1,m}]$ is a $\binom{m}{2} \times \binom{m}{3}$ matrix and the value of the the entry of $\mathbf{w}_{ijq}$ $(1 \le i < j < q \le m)$ will be 1 when exactly two of i-th, j-th and q-th factors are set to be 0. Otherwise, the value will be 0. Note that the 3 factors cannot all be '0' for the runs defined by $\mathbf{R}_m$. Hence, there are exactly 3 entries of each $\mathbf{w}_{ijq}$ vector that are 0, and the remaining entries are 1.

Performing the elementary column operations as described above on the matrix in (4), the resulting matrix is

$$\mathbf{M} = \begin{bmatrix} 1 & \mathbf{0}'_m & \mathbf{0}'_{\binom{m}{2}} & \mathbf{0}'_{\binom{m}{3}} \\ \mathbf{1}_m & \mathbf{I}_m & \mathbf{O} & \mathbf{O} \\ \mathbf{1}_{m(m-1)/2} & \mathbf{R}'_m & \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix}. \qquad (5)$$

From the structure of the matrix $\mathbf{M}$ and Theorem 2, we need to show that any selection of 4 columns from $[\mathbf{V}_1, \mathbf{V}_2]$ is of full column rank.

Define, for all $1 \leq i \leq (m-3)$,

$$\mathbf{P}_i = (\mathbf{q}_i * \mathbf{q}_{i+1}, \mathbf{q}_i * \mathbf{q}_{i+2}, \ldots, \mathbf{q}_i * \mathbf{q}_m),$$

$$\mathbf{P}_{m-2} = (\mathbf{q}_{m-2} * \mathbf{q}_{m-1}, \mathbf{q}_{m-2} * \mathbf{q}_m, \mathbf{q}_{m-1} * \mathbf{q}_m),$$

$$\mathbf{Q}_i = (\mathbf{q}_{i+1}, \mathbf{q}_{i+2}, \ldots, \mathbf{q}_m) \quad \text{and}$$

$$\mathbf{Q}_{m-2} = \mathbf{Q}_{m-3} = (\mathbf{q}_{m-2}, \mathbf{q}_{m-1}, \mathbf{q}_m).$$

Note that $\mathbf{V}_1 = [\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_{m-2}]$ and $\mathbf{Q}_1, \mathbf{Q}_2, \ldots, \mathbf{Q}_{m-2}$ are submatrices of $\mathbf{Q}' = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_m]$. The number of columns in $\mathbf{P}_i$ and $\mathbf{Q}_i$ is $m - i$, for $1 \leq i \leq (m-3)$. The number of columns in $\mathbf{P}_{m-2}$ and $\mathbf{Q}_{m-2}$ is 3.

In addition, we define B_1 to be the block of rows in $\mathbf{q}_1$ with values 0 and B_2 to be the block of rows in $\mathbf{q}_2$ with values 0 when those of $\mathbf{q}_1$ are 1. Similarly, we can define B_3 to be the block of rows in $\mathbf{q}_3$ with values 0 when those of $\mathbf{q}_1, \mathbf{q}_2$ are 1, and so on. It is easy to see that the number of rows in B_i is $m - i$, for $1 \leq i \leq (m-3)$, and the number of rows in B_{m-2} is 3. Also, for $1 \leq i \leq (m-3)$, the i-th diagonal block of $\mathbf{V}_1$ defined by B_i and $\mathbf{P}_i$ is a zero matrix of $(m-i) \times (m-i)$. The $(m-2)$th diagonal block of $\mathbf{V}_1$ defined by B_{m-2} and $\mathbf{P}_{m-2}$ is a zero matrix of 3×3.

Lemma 1. $\mathbf{V}_1$ *is a nonsingular matrix.*

From Lemma 1, it is clear that the proposed search design can be used to estimate all the main effects as well as all the two-factor interactions, if three- and higher-factor interactions are assumed to be absent.

4. Main theorem

We are going to use the following properties of the proposed search design:

- For any 4 columns selected, it is always possible to find rows with value 1. That is, we can always find a row vector $(1, 1, 1, 1)$ in the submatrix for $m \geq 5$.
- For any of the runs defined by $\mathbf{R}_m$, there are exactly two factors with level '0'; the remaining factors have level '1'. Specifically, the rows of $\mathbf{R}'_m$ can be identified by the set of index $\{i, j\}$ and the corresponding row is $\mathbf{r}'_{ij} = \mathbf{1}'_m - \mathbf{e}'_i - \mathbf{e}'_j$ with '0' in the i-th and j-th position and '1' in the other positions.
- $\mathbf{V}_1 = [\mathbf{v}_{12}, \ldots, \mathbf{v}_{m-1,m}]$ and the value of the entry of $\mathbf{v}_{ij}$ $(1 \leq i < j \leq m)$ will be 1 when both i-th and j-th factors are set to be 1. Otherwise, the value will be 0.
- As shown in Lemma 1, $\mathbf{V}_1$ is a full-rank matrix.

- $\mathbf{V}_2 = [\mathbf{w}_{123}, \ldots, \mathbf{w}_{m-2,m-1,m}]$ and the value of the the entry of $\mathbf{w}_{ijq}$ $(1 \le i < j < q \le m)$ will be 1 when exactly two of i-th, j-th and q-th factors are set to be 0. Otherwise, the value will be 0.

The following theorem shows that **Q** as defined in (3) satisfies Theorem 2 and thus can be used to estimate the grand mean and all main effects and correctly identify at least two of the interaction effects among all two- and three-factor interactions.

Theorem 3. *The columns of the matrix* **Q**, *interpreted as the level combinations of the factors* $F_1, F_2, \ldots, F_m$, *gives the required search design in N runs/level combinations.*

Theorem 3 suggests that the matrix **Q** presented in this section provides a search design in $N = 1 + m + m(m-1)/2$ runs, m being the number of factors involved which allow the estimation of the grand mean and all the main effects and allow the detection and estimation of at most two interactions among all the two- and three-factor interactions.

5. Conclusion

Much work has been done on the "main effect plus one" search design after the important work of Srivastava (1975). In this paper, we first give the necessary and sufficient conditions for the "main effect plus two" search design and then provide a new class of search designs that fulfills such a condition.

If a larger number of factors is under investigation and if only a small portion of interaction effects are expected (say, only two interaction effects are active among all two- and three-factor interactions), the search design given in this paper can be very useful.

To illustrate the run size issue, a brief run size comparison with a two-level Resolution VII plan is given in Table 1. Resolution VII is needed in order to estimate all two- and three-factor interactions. It is clear that the design in (3) can save a considerable experimental cost.

Table 1. Run size consideration for Resolution VII and search designs

Number of factors (m)	Resolution VII^{+} design	Design in (3)$^{++}$
5	32	16
6	64	22
7	64	29
8	128	37
9	256	46
10	256	56

$^{+}$ Resolution VII plan can estimate all main effects and all two- and three-factor interactions. (These run sizes are derived from Draper and Lin, 1990, Table 4.)

$^{++}$ Design in (3) can estimate all main effects and correctly identify two interaction effects.

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Appendix: Proofs

Proof of Lemma 1: Let $\mathbf{P}_i, \mathbf{Q}_i$ and B_i be as defined before.

Because of the construction of $\mathbf{Q}'$ (exactly two 0 in each row of $\mathbf{Q}'$), we have

$$\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \cdots + \mathbf{q}_m = (m-2)\mathbf{1}_{\binom{m}{2}}.$$

Therefore, for any $1 \le i \le m$, we have

$$\mathbf{q}_i * (\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \cdots + \mathbf{q}_m) = (m-2)\mathbf{q}_i.$$

Using the fact that $\mathbf{q}_i * \mathbf{q}_i = \mathbf{q}_i$, we have

$$\mathbf{q}_i * \left(\sum_{j \neq i} \mathbf{q}_j\right) / (m-3) = \mathbf{q}_i.$$

Hence, any column vector in $\mathbf{Q}'(\mathbf{q}_i)$ can be written as a linear combination of columns in $\mathbf{V}_1$. Therefore, the column transformations on $\mathbf{V}_1$ by columns in $\mathbf{Q}'$ will *not* affect the rank of $\mathbf{V}_1$.

Consider the following column transformation on $\mathbf{V}_1$ by columns in $\mathbf{Q}'$:

$$\mathbf{P}_i - \mathbf{Q}_i, \quad i = 1, \ldots, m-2.$$

Note that, for $i = m-2$, the $(m-2)$th block matrix of the matrix $\mathbf{P}_{m-2} - \mathbf{Q}_{m-2}$ is

$$\begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \equiv \mathbf{J}_{m-2},$$

which is a clearly a nonsingular matrix. Note also that, for $i = 1, \ldots, m-3$, we have

$$\mathbf{P}_i - \mathbf{Q}_i = ((\mathbf{q}_i - 1) * \mathbf{q}_{i+1}, (\mathbf{q}_i - 1) * \mathbf{q}_{i+2}, \ldots, (\mathbf{q}_i - 1) * \mathbf{q}_m).$$

The j-th block of the matrix $\mathbf{P}_i - \mathbf{Q}_i$ is a zero matrix for $i < j \le m$. The i-th block of the matrix $\mathbf{P}_i - \mathbf{Q}_i$ is $\mathbf{J}_i$, which is a $(m-i) \times (m-i)$ matrix with 0 on its diagonal and -1 for off-diagonal entries. Clearly, $\mathbf{J}_i$ is a nonsingular matrix.

Therefore, the resulting matrix is a block (upper) triangular matrix

$$\begin{pmatrix} \mathbf{J}_1 & * & * & * & * \\ \mathbf{O} & \mathbf{J}_2 & * & * & * \\ \mathbf{O} & \mathbf{O} & \ddots & * & * \\ \mathbf{O} & \mathbf{O} & \ddots & * & * \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{J}_{m-2} \end{pmatrix},$$

where the $\mathbf{J}_i$, $(1 \le i \le m-2)$, are block diagonal matrices which are all nonsingular matrices. Hence the matrix is a nonsingular matrix. □

Proof of Theorem 3: From the structure of the matrix $\mathbf{M}$ in (5), Theorem 3 can be proved if any selection of 4 columns from $[\mathbf{V}_1, \mathbf{V}_2]$ is of full column rank.

There are 5 cases in choosing 4 columns from matrix $[\mathbf{V}_1, \mathbf{V}_2]$: the number of columns chosen from $\mathbf{V}_1$ and $\mathbf{V}_2$ are $(4,0), (3,1), (2,2), (1,3)$, and $(0,4)$, respectively. In each case, we need to show that we can always find certain identified rows from the given 4 columns so that the submatrix has rank 4.

We will denote $C = A - B$ as the set of all elements in set A and not in set B.

Case 1: $\mathbf{X}_2^{**} = [\mathbf{v}_{i_1 j_1}, \mathbf{v}_{i_2 j_2}, \mathbf{v}_{i_3 j_3}, \mathbf{v}_{i_4 j_4}]$.

It follows easily from Lemma 1 that $\mathbf{V}_1$ is a full-rank matrix.

Case 2: $\mathbf{X}_2^{**} = [\mathbf{v}_{i_1 j_1}, \mathbf{v}_{i_2 j_2}, \mathbf{v}_{i_3 j_3}, \mathbf{w}_{i_4 j_4 q_4}]$.

Since $\{i_1, j_1\} \ne \{i_2, j_2\}$, we can always choose $i \in \{i_2, j_2\} - \{i_1, j_1\}$. Once i is chosen, we can choose j such that $j \notin \{i_1, j_1\}$ and $\{i, j\} \not\subset \{i_4, j_4, q_4\}$. Then, the row of $\mathbf{X}_2^{**}$ indexed by $\{i, j\}$ is

$$\begin{matrix} 1 & 0 & a & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3) & (i_4 j_4 q_4), \end{matrix}$$

where a can be 0 or 1.

Similarly, choose $i \in \{i_1, j_1\} - \{i_2, j_2\}$. Once i is chosen, we can choose j such that $j \notin \{i_2, j_2\}$ and $\{i, j\} \not\subset \{i_4, j_4, q_4\}$. Then, the row of $\mathbf{X}_2^{**}$ indexed by $\{i, j\}$ is

$$\begin{matrix} 0 & 1 & b & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3) & (i_4 j_4 q_4), \end{matrix}$$

where b can be 0 or 1.

Applying the same argument for sets $\{i_1, j_1\}$ and $\{i_3, j_3\}$, we can find two rows

$$\begin{array}{cccc} 0 & c & 1 & 1 \\ 1 & d & 0 & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3) & (i_4 j_4 q_4), \end{array}$$

where c, d can be 0 or 1.

Therefore, we have identified the following rows

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & a & 1 \\ 0 & 1 & b & 1 \\ 0 & c & 1 & 1 \\ 1 & d & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

Clearly, $\mathbf{S}$ has rank 4 if and only if $f(a,b,c,d) = \det(\mathbf{S}'\mathbf{S}) \neq 0$. In fact,

$$\begin{aligned} f(a,b,c,d) = {} & a^2(2c^2 - 4c + 2d^2 - 4d + 4) \\ & - 2a(b(c-1)(d+1) + c^2 - c(d+3) + 2d^2 - d + 2) \\ & + 2b^2(d^2 - d + 1) - 2b(c(d-2) + 2d^2 - 3d + 4) \\ & + 2c^2 + c(2d - 8) + 4d^2 - 4d + 8. \end{aligned}$$

It can be shown that $\mathbf{S}$ has rank 4 for all 2^4 choices of (a,b,c,d), except the combination $(a,b,c,d) = (0,1,1,0)$. When $(a,b,c,d) = (0,1,1,0)$, however, $\mathbf{S}$ becomes

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

We can remove the two duplicated rows (3rd and 4th) and add an additional row from sets $\{i_2, j_2\}$ and $\{i_3, j_3\}$ (using a similar argument as above):

$$\begin{array}{cccc} e & 0 & 1 & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3) & (i_4 j_4 q_4), \end{array}$$

where e can be 0 or 1. Therefore, we have the following submatrix

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ e & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

with $\det(\mathbf{S}) = -1$ which does not depend on the value of e.

Case 3: $\mathbf{X}_2^{**} = [\mathbf{v}_{i_1 j_1}, \mathbf{v}_{i_2 j_2}, \mathbf{w}_{i_3 j_3 q_3}, \mathbf{w}_{i_4 j_4 q_4}]$.

We can choose $i \in \{i_2, j_2\} - \{i_1, j_1\}$ and then choose j such that $j \notin \{i_1, j_1\}$, $\{i, j\} \not\subset \{i_3, j_3, q_3\}$ and $\{i, j\} \not\subset \{i_4, j_4, q_4\}$. Then, the row of $\mathbf{X}_2^{**}$ indexed by $\{i, j\}$ is

$$\begin{matrix} 1 & 0 & 1 & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4). \end{matrix}$$

Similarly, by symmetry, we can find the row

$$\begin{matrix} 0 & 1 & 1 & 1 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4). \end{matrix}$$

Finally, we choose $i \in \{i_4, j_4, q_4\} - \{i_3, j_3, q_3\}$ and then choose j such that $\{i, j\} \subset \{i_4, j_4, q_4\}$. Then, the row of $\mathbf{X}_2^{**}$ indexed by $\{i, j\}$ is

$$\begin{matrix} a & b & 1 & 0 \\ (i_1 j_1) & (i_2 j_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4), \end{matrix}$$

where a, b can be 0 or 1. Therefore, we have found a submatrix

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ a & b & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

whose determinant is always 1, independent of the values of a, b.

Case 4: $\mathbf{X}_2^{**} = [\mathbf{v}_{i_1 j_1}, \mathbf{w}_{i_2 j_2 q_2}, \mathbf{w}_{i_3 j_3 q_3}, \mathbf{w}_{i_4 j_4 q_4}]$.

If we choose $i \in \{i_1, j_1\}$ and j such that $\{i, j\} \not\subset \{i_2, j_2, q_2\}$, $\{i, j\} \not\subset \{i_3, j_3, q_3\}$, $\{i, j\} \not\subset \{i_4, j_4, q_4\}$, we can find a row

$$\begin{matrix} 0 & 1 & 1 & 1 \\ (i_1 j_1) & (i_2 j_2 q_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4). \end{matrix}$$

Next, choose $\{i, j\}$ such that $\{i, j\} \subset \{i_2, j_2, q_2\}$, $\{i, j\} \not\subset \{i_3, j_3, q_3\}$, and $\{i, j\} \not\subset \{i_4, j_4, q_4\}$, we can find a row

$$\begin{matrix} a & 0 & 1 & 1 \\ (i_1 j_1) & (i_2 j_2 q_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4), \end{matrix}$$

where a can be 0 or 1. Similarly, choose $\{i, j\}$ such that $\{i, j\} \subset \{i_3, j_3, q_3\}$, $\{i, j\} \not\subset \{i_2, j_2, q_2\}$, and $\{i, j\} \not\subset \{i_4, j_4, q_4\}$, we can find a row

$$\begin{matrix} b & 1 & 0 & 1 \\ (i_1 j_1) & (i_2 j_2 q_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4). \end{matrix}$$

Hence, we have found a submatrix

$$\mathbf{S} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ a & 0 & 1 & 1 \\ b & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

whose determinant is always 1, independent of the values of a, b.

Case 5: $\mathbf{X}_2^{**} = [\mathbf{w}_{i_1 j_1 q_1}, \mathbf{w}_{i_2 j_2 q_2}, \mathbf{w}_{i_3 j_3 q_3}, w_{i_4 j_4 q_4}]$.

We need to consider two subcases (complementary to each other):

(5-a) $\{i_1, j_1, q_1\}$ has at most one element in common with some of the sets $\{i_2, j_2, q_2\}$, $\{i_3, j_3, q_3\}$, $\{i_4, j_4, q_4\}$.

(5-b) $\{i_1, j_1, q_1\}$ has two elements in common with each of the sets $\{i_2, j_2, q_2\}$, $\{i_3, j_3, q_3\}$, $\{i_4, j_4, q_4\}$.

For subcase (5-a), without loss of generality (rearrange the columns, if necessary), assume that $\{i_4, j_4, q_4\}$ and $\{i_1, j_1, q_1\}$ have at most one element in common. In this case, choose $\{i, j\}$ such that $\{i, j\} \subset \{i_1, j_1, q_1\}$, $\{i, j\} \not\subset \{i_2, j_2, q_2\}$, $\{i, j\} \not\subset \{i_3, j_3, q_3\}$, and, because of the condition that $\{i_4, j_4, q_4\}$ and $\{i_1, j_1, q_1\}$ can't have two elements in common, $\{i, j\} \not\subset \{i_4, j_4, q_4\}$. Therefore, we find a row

$$\begin{matrix} 0 & 1 & 1 & 1 \\ (i_1 j_1 q_1) & (i_2 j_2 q_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4). \end{matrix}$$

Next, using a similar argument as in Case 4, we can also find two rows with

$$\begin{matrix} a & 0 & 1 & 1 \\ b & 1 & 0 & 1 \\ (i_1 j_1 q_1) & (i_2 j_2 q_2) & (i_3 j_3 q_3) & (i_4 j_4 q_4), \end{matrix}$$

where a and b can be 0 or 1. Therefore, we find a submatrix

$$\mathbf{S} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ a & 0 & 1 & 1 \\ b & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

whose determinant is always 1, independent on the values of a, b.

For subcase (5-b), we need to further divide the argument into three parts depending on the value of s, which is the maximum number satisfying the condition that the intersection of the set $\{i_1, j_1, q_1\}$ with the intersection of s sets taken from $[\{i_2, j_2, q_2\}, \{i_3, j_3, q_3\}, \{i_4, j_4, q_4\}]$ is a non-empty set with *two* elements. Clearly, under (5-b), $1 \leq s \leq 3$.

Without loss of generality (rearrange the columns, if necessary), we may assume the sets corresponding to s are adjacent to $\{i_1, j_1, q_1\}$.

– If $s=1$, then $Z=\{i_1,j_1,q_1\}\cap\{i_2,j_2,q_2\}$ is non-empty (hence, with 2 elements), $Z\not\subset\{i_3,j_3,q_3\}$, and $Z\not\subset\{i_4,j_4,q_4\}$. Therefore, choosing $\{i,j\}=\{i_1,j_1,q_1\}\cap\{i_2,j_2,q_2\}$ will yield a row with $(0,0,1,1)$. Similarly, choosing $\{i,j\}=\{i_1,j_1,q_1\}\cap\{i_3,j_3,q_3\}$ will yield a row with $(0,1,0,1)$. Finally, choosing $\{i,j\}=\{i_1,j_1,q_1\}\cap\{i_4,j_4,q_4\}$ will yield a row with $(0,1,1,0)$. Therefore, we find a submatrix

$$\mathbf{S}=\begin{bmatrix}0&0&1&1\\0&1&0&1\\0&1&1&0\\1&1&1&1\end{bmatrix}$$

whose determinant is -1.

– If $s=2$, then $Z=\{i_1,j_1,q_1\}\cap\{i_2,j_2,q_2\}\cap\{i_3,j_3,q_3\}$ is a non-empty set with exactly two elements. Choosing $\{i,j\}=Z$, we have a row $(0,0,0,1)$. Next, choosing $i\in Z$ and then $j\in\{i_2,j_2,q_2\}-\{i_1,j_1,q_1\}$ will yield a row $(1,0,1,a)$, where a can be 0 or 1. Similarly, choosing $i\in Z$ and then $j\in\{i_3,j_3,q_3\}-\{i_1,j_1,q_1\}$ will yield a row $(1,1,0,b)$, where b can be 0 or 1. Therefore, we find a submatrix

$$\mathbf{S}=\begin{bmatrix}0&0&0&1\\1&0&1&a\\1&1&0&b\\1&1&1&1\end{bmatrix}$$

whose determinant is always -1, independent on the values of a,b.

– If $s=3$, then $Z=\{i_1,j_1,q_1\}\cap\{i_2,j_2,q_2\}\cap\{i_3,j_3,q_3\}\cap\{i_4,j_4,q_4\}$ is non-empty with two elements. In this case, choosing $i\in\{i_1,j_1,q_1\}-Z$ and then $j\in Z-\{i\}$ will yield a row $(0,1,1,1)$. By symmetry, we can find three other rows $(1,0,1,1)$, $(1,1,0,1)$, and $(1,1,1,0)$. Therefore, we found a submatrix

$$\mathbf{S}=\begin{bmatrix}0&1&1&1\\1&0&1&1\\1&1&0&1\\1&1&1&0\end{bmatrix}$$

whose determinant is -3.

We have shown in Case 1–Case 5 that we can indeed find a submatrix of $\mathbf{X}_2^{**}$ which is of rank 4. Thus, the proof of Theorem 3 is complete. □