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Variance exchange process: overcoming the problem of singular information matrices in quadratic three-variable response designs

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Abstract. Many times, in a variance exchange process for identifying D-optimal designs, the initial designs of all quadratic components of three-variable response polynomials yield non-invertible information matrices. For such matrices, the variances of predicted responses at the design points cannot be evaluated, making the variance exchange process impossible. D-optimality is a design criterion that seeks to maximize the determinant of the information matrix, or equivalently, minimize the determinant of the inverse information matrix of the design. This work addresses the challenges posed by initial quadratic designs with zero-determinant information matrices for three-variable response polynomials, enabling the possibility of variance exchange.

The singular value decomposition (SVD) method was adopted, and an algorithm was developed for a variance exchange process involving quadratic designs of three-variable response functions. The study analyzed generated data for quadratic three-variable designs of sizes 12 and 13. MATLAB 7.5.0 (R2007b) was used to compute the Penrose inverses.

The results demonstrate that a variance exchange process is feasible, allowing the evaluation of the variances of predicted responses at the design points and overcoming the issue of singular information matrices in the initial quadratic designs.

The D-optimal designs, or computer-generated optimal designs, offer practical alternatives for determining optimal conditions for factors in engineering optimization problems. These designs are particularly useful for response surface functions requiring structured data collection through experimental design when the experimental design space is constrained due to the zero determinant of the information matrices in the initial designs.

Keywords: Variance Exchange Process, Three-variable Quadratic Designs, Singular Information Matrix, Generalized Inverse.).

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1 Introduction

The variance exchange process, an algorithmic search procedure for constructing exact D-optimum designs as described in [4] and [9], depends on the variance of the predicted responses at the design points $\mathbf{x}_i' M^{-1}\{\xi_N\}\mathbf{x}_i$, the determinant $\det M(\xi_N)$ of the design's information matrix, and the values of the elements of its inverse $M^{-1}(\xi_N)$.

The inverse of a design matrix is defined only for square, nonsingular matrices. A common situation in statistics, as well as in many other fields of application, involves solving a system of linear equations, such as in Equation (1.1) [11]:

$$A\mathbf{x} = \boldsymbol{c}. \tag{1.1}$$

In Equation (1.1), A is an $m \times n$ matrix of constants, $\boldsymbol{c}$ is an $m \times 1$ vector of constants, and $\mathbf{x}$ is an $n \times 1$ vector of variables for which solutions are sought. Such solutions are possible only if $m = n$ and A is nonsingular, in which case the inverse A^{-1} exists. The system in Equation (1.1) is satisfied only when $\mathbf{x} = A^{-1}\mathbf{c}$, resulting in a unique solution. Here, A is said to be of full rank. If, however, A is not of full rank and A^{-1} does not exist, the system in Equation (1.1) has no solution.

The variance exchange process can only proceed when the information matrix of a design is nonsingular, i.e., $M\{\xi_N\} = X'X$ is of full rank, and the predicted variances of the design points, $\mathbf{x}_i' M^{-1}\{\xi_N\}\mathbf{x}_i$, can be computed. This dependency arises because the rank of a matrix determines its invertibility: a matrix with less-than-full rank is not invertible, and its determinant is zero.

In the case of a three-variable response function, the initial designs for all quadratic components are of less-than-full rank and consequently produce singular information matrices, $M(\xi_N^{(1)})$. Specifically, $r\{X'X\} < c$, where c is the number of columns, and $\mathbf{x}_i' M^{-1}\{\xi_N\}\mathbf{x}_i$ cannot be evaluated. As a result, the variance exchange process is not feasible when the degree of the three-variable response function includes quadratic terms.

[1] has noted that, in a variance exchange process, if a design matrix ξ_N or its information matrix $M(\xi_N) = (X'X)$ has a zero determinant, the inverse information matrix cannot be computed. Furthermore, [3] observed that while good starting designs might be available, they do not necessarily guarantee designs with maximum determinants. Similarly, [6] and [2] pointed out that starting designs can sometimes be singular. In their work, "On the Difference in Cycling Pattern on Linear and Higher-Order Effect Designs," [10] found that starting designs for all quadratic components of three-variable second-order polynomials have singular information matrices, thus preventing a variance exchange process.

In this study, we address the challenges posed by zero-determinant information matrices in initial quadratic designs for a three-variable response polynomial function. Our primary aim is to compute a unique Penrose inverse $G = (X'X)^+$ for the singular quadratic information matrix $(X'X)$, evaluate the predicted response variances $\mathbf{x}_i'(X'X)^+\mathbf{x}_i$ at design points, and construct an algorithm to enable the variance exchange process for initial designs with singular information matrices.

2 Materials and methods

In a variance exchange process, the variance of predicted responses at design points, $\mathbf{x}_i' M^{-1}\{\xi_N\}\mathbf{x}_i$, can only be evaluated for nonsingular information matrices. The information matrix, $M\{\xi_N\}$, for a quadratic three-variable design is singular. To assess these variances of predicted responses, a generalized inverse $(X'X)^-$ is required. However, several different generalized inverses of $M\{\xi_N\}$ exist, meaning $(X'X)^-$ is not unique. To address this, we adopt the Moore-Penrose inverse, a unique pseudoinverse for singular information matrices, as outlined by [12] and [13], to assess the predicted variances. Using this pseudoinverse, we constructed an algorithm to overcome the problem of zero determinants, ultimately making the variance exchange process workable for a three-variable quadratic information matrix.

2.1 The Moore-Penrose inverse

Let $\xi_N^{(1)}$ be an initial N-point design measure, and let X be the corresponding design matrix. Then, according to [11] and [12], the Moore-Penrose inverse is defined as follows:

Definition 2.1. The Moore-Penrose inverse of X, denoted by X^+, satisfies the conditions:

$$X(X^+)X = X, \tag{2.1}$$

$$(X^+)X(X^+) = X^+, \tag{2.2}$$

$$[X(X^+)]' = X(X^+), \tag{2.3}$$

$$[(X^+)X]' = (X^+)X. \tag{2.4}$$

The pseudoinverse, as described by [13], provides a "best fit" solution for non-square or singular matrices that do not have a standard inverse. According to [11], it is a generalization of spectral factorization to non-symmetric matrices, known as the singular value decomposition (SVD), defined as:

Definition 2.2. If $X = R\mathbf{\Sigma}S'$ is the singular value decomposition of the N-point design matrix X, then its pseudoinverse is given by $X^+ = S\mathbf{\Sigma}^{-1}R'$.

For theoretical purposes, [7], as cited by [12], provided an expression to compute the Moore-Penrose inverse of a partitioned $m \times n$ matrix X recursively. Let $X_i = (\mathbf{x}_1, ..., \mathbf{x}_i)$, where $\mathbf{x}_i$ denotes the i-th column of X, so that X_i is the $m \times i$ matrix containing the first i columns of X. Greville showed that if we write $X_i = [X_{i-1}\ \mathbf{x}_i]$ $(i = 2, \ldots, n)$, then:

$$X_i^+ = [X_{i-1}\ \mathbf{x}_i]^+ = \begin{bmatrix} X_{i-1}^+ - d_i b_i' \\ b_i' \end{bmatrix}, \tag{2.5}$$

where:

$$b_i' = \begin{cases} (c_i' c_i)^{-1} c_i', & \text{if } c_i \neq 0, \\ (1 + d_i' d_i)^{-1} d_i' X_{i-1}^+, & \text{if } c_i = 0, \end{cases}$$

and the vectors d_i and c_i are defined as:

$$d_i = X_{i-1}^+ \mathbf{x}_i,$$
$$c_i = \mathbf{x}_i - X_{i-1} d_i = \mathbf{x}_i - A_{i-1} X_{i-1}^+ \mathbf{x}_i.$$

Thus, $X^+ = X_n^+$ can be computed successively by calculating $X_2^+, X_3^+, ..., X_n^+$.

Stanimirovic [14] proposed an algorithm based on Equation (2.5) for computing the Moore-Penrose inverse as follows:

Start: For an arbitrary $m \times n$ matrix X, compute:

$$X_1^+ = \mathbf{x}_1^+ = \begin{cases} (\mathbf{x}_1'\mathbf{x}_1)^{-1}\mathbf{x}_1', & \mathbf{x}_1 \neq 0, \\ 0, & \mathbf{x}_1 = 0. \end{cases}$$

For $i = 2$ to n, do:

$$d_i := X_{i-1}^+ \mathbf{x}_i,$$
$$c_i := \mathbf{x}_i - X_{i-1} d_i.$$

If $c_i \neq 0$, compute:

$$b_i' := \left(c_i' c_i\right)^{-1} c_i'.$$

Otherwise:

$$b_i' := \left(1 + d_i' d_i\right)^{-1} d_i' X_{i-1}^+.$$

Then:

$$X_i^+ = \begin{bmatrix} X_{i-1}^+ - d_i b_i' \\ b_i' \end{bmatrix}.$$

Repeat until $X^+ = X_n^+$.

2.2 Algorithm to overcome information matrix singularities in a quadratic level variance exchange process for a three-variable design

Given an initial N-point design matrix $X = \xi_N^{(1)}$ from a candidate set $\widetilde{N}$ obtained from a metric space of factor levels $\widetilde{X}$, a variance exchange is possible if the matrix $M(\xi_N^{(1)})$ is nonsingular and invertible for linear, mixed, and quadratic portions of the three-variable response situation [9].

For an initial quadratic component three-variable singular and noninvertible information matrix $M(\xi_N^{(1)})$, the structure of the variance exchange process is defined by the following iterative steps:

(I) Determine the Moore-Penrose generalized inverse of the singular information matrix $M(\xi_N^{(1)})$.

(II) Compute the variances $d\left(\mathbf{x}_v, \xi_N^{(1)}\right)$ for points within the design $\xi_N^{(1)}$ and $d\left(\mathbf{x}_w, \xi_N^{(1)}\right)$ for points in the complement design $\xi_N^{(1)c}$:

$$d\left(\mathbf{x}_v, \xi_N^{(1)}\right) = \min_{\mathbf{x} \in X_N^{(1)}} \mathbf{x}'_i (X'X)^+ \mathbf{x}_i, \tag{2.6}$$

$$d\left(\mathbf{x}_w, \xi_N^{(1)}\right) = \max_{\mathbf{x} \in X_N^{(1)c}} \mathbf{x}_j' (X'X)^+ \mathbf{x}_j. \tag{2.7}$$

(III) Compare Equations (2.6) and (2.7), the minimum and maximum variances of the design and its complement.

If $d\left(\mathbf{x}_w, \xi_N^{(1)}\right) \leq d\left(\mathbf{x}_v, \xi_N^{(1)}\right)$, stop. Otherwise, exchange the point with the minimum variance in $\xi_N^{(1)}$ with the point with the maximum variance from $\xi_N^{(1)c}$, the complement design. Define a new design measure and repeat step (II) until $d\left(\mathbf{x}_w, \xi_N^{(k)}\right) \leq d\left(\mathbf{x}_v, \xi_N^{(k)}\right)$.

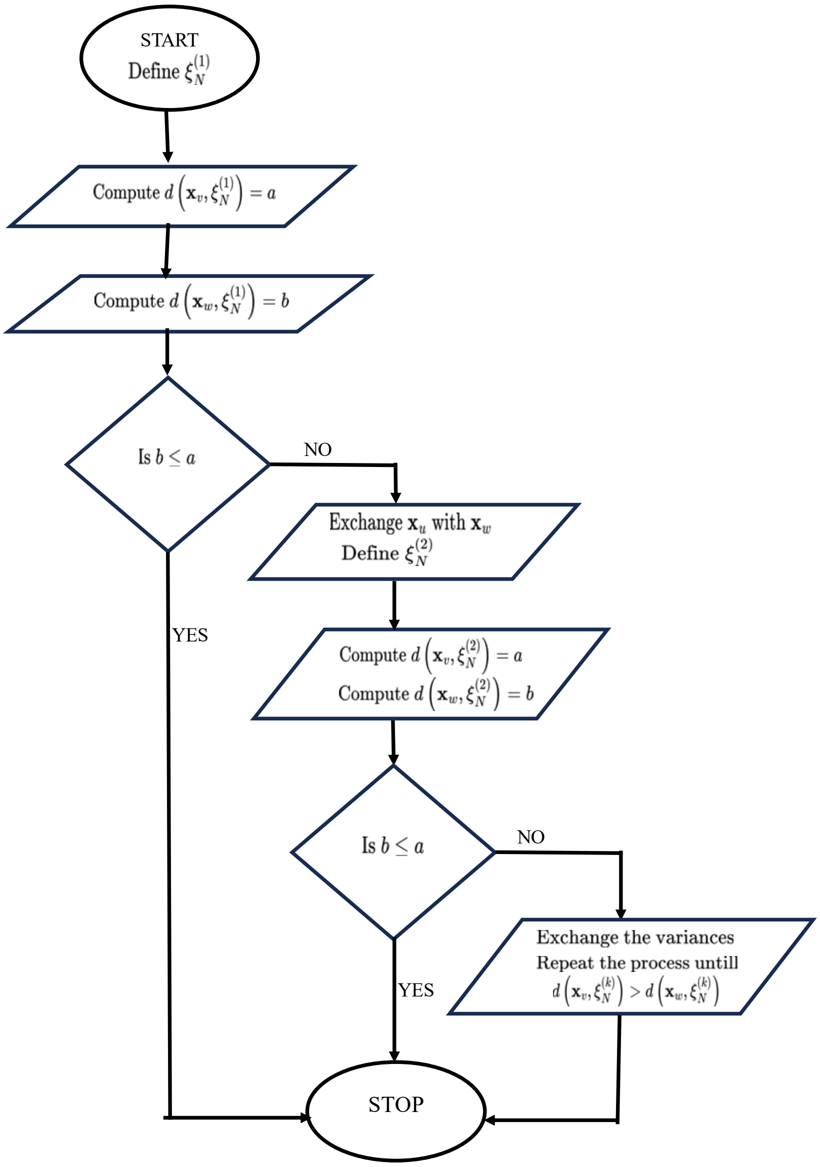

Figure 2.1: Flowchart describing the algorithm.

Figure 2.1 provides a flowchart illustrating the stated algorithm.

The algorithm terminates when no further exchange increases the determinant, indicating that the determinant of the information matrix is at its maximum. That is,

$$\left|M\left(\xi_X^{(k)}\right)\right| = \left|M\left(\xi_X^{(\star)}\right)\right|,$$

where $\xi_X^{(\star)}$ is the desired exact D-optimal design measure.

However, this procedure may not always converge to the best exact D-optimal design due to what [8] describes as cycling. When cycling occurs in the sequential process, the determinant of the information matrix stagnates, leading to:

$$d\left(\mathbf{x}_w, \xi_N^{(k)}\right) > d\left(\mathbf{x}_v, \xi_N^{(k-1)}\right) \text{ and } \left|M\left(\xi_N^{(k)}\right)\right| \leq \left|M\left(\xi_N^{(k-1)}\right)\right|.$$

The effects of cycling include:

(i) The absence of a defined maximum determinant.

(ii) Failure to converge to D-optimality:

$$M\left(\xi_N^{(1)}\right) \leq M\left(\xi_N^{(2)}\right) \leq \cdots \leq M\left(\xi_N^{(k)}\right) \leq \cdots \leq M\left(\xi_N^{(\star)}\right).$$

3 Analysis and results

The statistical analysis employs the model in Equation (3.1), a three-variable quadratic response polynomial function. Both even- and odd-sized designs are considered to evaluate the impact of zero determinants on designs. Specifically, designs of sizes 12 and 13 are analyzed.

$$f(x_1, x_2, x_3) = a_0 + \sum_{i=1}^{3} a_i x_i + \sum_{i=1}^{3} a_{ii} x_i^2 + \sum_{i<j}\sum a_{ij} x_i x_j + \mathbf{e}, \tag{3.1}$$

where a_0 is the intercept, a_i are the linear coefficients, a_{ii} are the quadratic coefficients, a_{ij} are the interaction coefficients, and $\mathbf{e}$ represents the error term.

The experimental space used to generate data for designs of sizes 12 and 13 points is defined as:

$$\widetilde{X} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 : \mathbf{x}_1 = -2, -1, 1, 2; \mathbf{x}_2 = -1, 0, 1; \mathbf{x}_3 = -1, 1\},$$

with $E(\mathbf{e}) = 0$ and $Var(\mathbf{e}) = \sigma_e^2$.

3.1 The three-variable, quadratic 12-point designs

The initial and complement design matrices for the three-variable quadratic 12-point design are as follows:

$$X_{12}^{(1)} = \begin{pmatrix}
1 & -2 & -1 & -1 & 4 & 1 & 1 & 2 & 2 & 1 \\
1 & -2 & 0 & 1 & 4 & 0 & 1 & 0 & -2 & 0 \\
1 & -2 & 1 & -1 & 4 & 1 & 1 & -2 & 2 & -1 \\
1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 \\
1 & -1 & 0 & 1 & 1 & 0 & 1 & 0 & -1 & 0 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 0 & -1 & 1 & 0 & 1 & 0 & -1 & 0 \\
1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\
1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\
1 & 2 & -1 & -1 & 4 & 1 & 1 & -2 & 2 & 1 \\
1 & 2 & 0 & -1 & 4 & 0 & 1 & 0 & -2 & 0 \\
1 & 2 & 0 & 1 & 4 & 0 & 1 & 0 & 2 & 0
\end{pmatrix}$$

$$X_{12}^{(1)c} = \begin{pmatrix} 1 & -2 & -1 & 1 & 4 & 1 & 1 & 2 & -2 & -1 \\ 1 & -2 & 0 & -1 & 4 & 0 & 1 & 0 & 2 & 0 \\ 1 & -2 & 1 & 1 & 4 & 1 & 1 & -2 & -2 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 0 & -1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & 1 & 4 & 1 & 1 & -2 & 2 & -1 \\ 1 & 2 & 1 & -1 & 4 & 1 & 1 & 2 & -2 & -1 \\ 1 & 2 & 1 & 1 & 4 & 1 & 1 & 2 & 2 & 1 \end{pmatrix}$$

The information matrix and its determinant are given as:

$$M\left\{\xi_{12}^{(1)}\right\} = \begin{pmatrix} 12 & 0 & 0 & -2 & 30 & 6 & 12 & -1 & -2 & -2 \\ 0 & 30 & -1 & -2 & 0 & -3 & 0 & -3 & -8 & 3 \\ 0 & -1 & 6 & -2 & -3 & 0 & 0 & -3 & 3 & -4 \\ -2 & -2 & -2 & 12 & -8 & -4 & -2 & 3 & 0 & 0 \\ 30 & 0 & -3 & -8 & 102 & 15 & 30 & -7 & -2 & 1 \\ 6 & -3 & 0 & -4 & 15 & 6 & 6 & -1 & 1 & -2 \\ 12 & 0 & 0 & -2 & 30 & 6 & 12 & -1 & -2 & -2 \\ -1 & -3 & -3 & 3 & -7 & -1 & -1 & 15 & 1 & 1 \\ -2 & -8 & 3 & 0 & -2 & 1 & -2 & 1 & 30 & -1 \\ -2 & 3 & -4 & 0 & 1 & -2 & -2 & 1 & -1 & 6 \end{pmatrix}$$

$$\text{Det}\left\{M\left(\xi_{12}^{(1)}\right)\right\} = 0$$

Since the determinant is zero, the 10×10 information matrix $M(\xi_{12}^{(1)})$ is singular and non-invertible. Consequently, the variances of the predicted responses, $\mathbf{x}_i' M^{-1}\{\xi_{12}^{(1)}\}\mathbf{x}_i$, cannot be evaluated directly.

To address this, we employ singular value decomposition (SVD) to determine the Moore-Penrose pseudoinverse of $M(\xi_{12}^{(1)})$, enabling the computation of variances $\mathbf{x}_i' M^{-1}\{\xi_{12}^{(1)}\}\mathbf{x}_i$. MATLAB 7.5.0 (R200b) provides the SVD of $M(\xi_{12}^{(1)})$ as:

$$\text{svd}\left\{M\left(\xi_{12}^{(1)}\right)\right\} = \begin{pmatrix} 124.4755 \\ 39.0867 \\ 23.1874 \\ 17.0400 \\ 11.0782 \\ 10.1217 \\ 3.8464 \\ 1.6959 \\ 0.4683 \\ 0.0000 \end{pmatrix}$$

The $[U, \Sigma, V] = \text{svd}\left\{M\left(\xi_{12}^{(1)}\right)\right\}$ gives:

$$U = \begin{pmatrix} -0.280 & 0.004 & -0.066 & -0.004 & 0.238 & -0.294 & -0.276 & 0.434 & 0.097 & 0.707 \\ -0.002 & 0.709 & 0.619 & 0.236 & 0.141 & -0.158 & -0.027 & -0.103 & -0.038 & 0.000 \\ 0.020 & -0.082 & 0.139 & -0.356 & 0.192 & -0.310 & 0.622 & 0.229 & -0.524 & 0.000 \\ 0.081 & -0.037 & -0.199 & 0.406 & -0.523 & -0.653 & -0.074 & -0.116 & -0.264 & 0.000 \\ -0.900 & -0.024 & 0.034 & 0.115 & -0.200 & 0.117 & 0.281 & -0.207 & 0.000 & 0.000 \\ -0.145 & -0.093 & -0.028 & -0.152 & 0.306 & 0.044 & -0.526 & -0.432 & -0.622 & 0.000 \\ -0.280 & 0.004 & -0.066 & -0.004 & 0.238 & -0.294 & -0.276 & 0.434 & 0.097 & -0.707 \\ 0.066 & -0.097 & -0.271 & 0.701 & 0.575 & 0.075 & 0.278 & -0.066 & -0.062 & 0.000 \\ 0.018 & -0.679 & 0.687 & 0.224 & -0.004 & -0.045 & -0.095 & 0.031 & 0.063 & 0.000 \\ 0.004 & 0.096 & 0.041 & 0.276 & -0.302 & 0.507 & -0.112 & 0.558 & -0.491 & 0.000 \end{pmatrix},$$

$$\Sigma = \begin{pmatrix} 124.476 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 39.087 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 23.187 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 17.040 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 11.078 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10.122 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3.846 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.696 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.468 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 \end{pmatrix}.$$

$$V = \begin{pmatrix} -0.280 & 0.004 & -0.066 & -0.004 & 0.238 & -0.294 & -0.276 & 0.434 & 0.097 & 0.707 \\ -0.002 & 0.709 & 0.619 & 0.236 & 0.141 & -0.156 & -0.027 & -0.103 & -0.038 & 0.000 \\ 0.020 & -0.082 & 0.139 & -0.356 & 0.192 & -0.310 & 0.622 & 0.229 & -0.524 & 0.000 \\ 0.081 & -0.037 & -0.198 & 0.406 & -0.523 & -0.653 & -0.074 & -0.116 & -0.264 & 0.000 \\ -0.900 & -0.024 & 0.034 & 0.115 & -0.200 & 0.117 & 0.281 & -0.207 & 0.000 & 0.000 \\ -0.145 & -0.093 & -0.028 & -0.152 & 0.306 & 0.044 & -0.526 & -0.432 & -0.622 & 0.000 \\ -0.280 & 0.004 & -0.066 & -0.004 & 0.238 & -0.294 & -0.276 & 0.434 & 0.097 & -0.707 \\ 0.066 & -0.097 & -0.271 & 0.701 & 0.575 & 0.075 & 0.278 & -0.066 & -0.062 & 0.000 \\ 0.031 & -0.679 & 0.687 & 0.224 & -0.004 & -0.045 & -0.095 & 0.031 & 0.063 & -0.000 \\ 0.004 & 0.096 & 0.041 & 0.276 & -0.302 & 0.507 & -0.112 & 0.558 & -0.491 & 0.000 \end{pmatrix}.$$

From these results, it is established that:

(i) $M\left(\xi_{12}^{(1)}\right) = U\mathbf{\Sigma}V'$,

(ii) The Penrose inverse of $(X'X)$, $(X'X)^{+} = V\mathbf{\Sigma}^{-1}U'$.

The variances evaluated from $\mathbf{x}_i'\left(X'X\right)^{+}\mathbf{x}_i$ are shown in Table 3.1.

3.2 The three-variable, quadratic 13-point designs

The initial and complement design matrices for the three-variable quadratic 13-point design are as follows:

Table 3.1: Variances of points for the initial two-variable linear 12-point designs

Vector	Current Design		Complement Design	
	Vector Point	Var	Vector Point	Var
$\mathbf{x_1}$	(1 − 2 − 1 − 1 4 1 1 2 2 1)	0.9950	(1 − 2 − 1 1 4 1 1 2 − 1 − 1)	1.7212
$\mathbf{x_2}$	(1 − 2 0 1 4 0 1 0 − 2 1)	1.7804	(1 − 2 0 − 1 4 0 1 0 2 0)	1.5106
$\mathbf{x_3}$	(1 − 2 1 − 1 4 1 1 − 2 2 − 1)	0.7738	(1 − 2 1 1 4 1 1 − 2 − 2 1)	6.7847
$\mathbf{x_4}$	(1 − 1 − 1 1 1 1 1 1 − 1 − 1)	1.0000	(1 − 1 − 1 − 1 1 1 1 1 1 1)	1.1109
$\mathbf{x_5}$	(1 − 1 0 1 1 0 1 0 − 1 0)	0.4807	(1 − 1 0 − 1 1 0 1 0 1 0)	1.2956
$\mathbf{x_6}$	(1 − 1 1 − 1 1 1 1 − 1 1 − 1)	0.4440	(1 − 1 1 1 1 1 1 − 1 − 1 1)	6.8866
$\mathbf{x_7}$	(1 1 0 − 1 1 0 1 0 − 1 0)	0.6775	(1 1 − 1 − 1 1 1 1 − 1 − 1 1)	1.1825
$\mathbf{x_8}$	(1 1 0 1 1 0 1 0 1 0)	0.4897	(1 1 − 1 1 1 1 1 − 11 − 1)	1.7740
$\mathbf{x_9}$	(1 1 1 − 1 1 1 1 1 − 1 − 1)	0.9143	(1 1 1 1 1 1 1 1 1 1)	7.1562
$\mathbf{x_{10}}$	(1 2 − 1 − 1 4 1 1 − 2 − 2 1)	0.9950	(1 2 − 1 1 4 1 1 1 − 2 2 − 1)	2.8546
$\mathbf{x_{11}}$	(1 2 0 − 1 4 0 1 0 − 2 0)	0.6775	(1 2 1 − 1 4 1 1 1 2 − 2 − 1)	2.6641
$\mathbf{x_{12}}$	(1 2 0 1 4 0 1 0 2 0)	0.7807	(1 2 1 1 4 1 1 2 1)	7.8704

$$X_{13}^{(1)} = \begin{pmatrix} 1 & -2 & -1 & 1 & 4 & 1 & 1 & 2 & -2 & -1 \\ 1 & -2 & 0 & -1 & 4 & 0 & 1 & 0 & 2 & 0 \\ 1 & -1 & 0 & -1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 2 & -1 & -1 & 4 & 1 & 1 & -2 & 2 & 1 \\ 1 & 2 & -1 & 1 & 4 & 1 & 1 & -2 & 2 & -1 \\ 1 & 2 & 0 & 1 & 4 & 0 & 1 & 0 & 2 & 0 \\ 1 & 2 & 1 & -1 & 4 & 1 & 1 & 2 & -2 & -1 \\ 1 & 2 & 1 & 1 & 4 & 1 & 1 & 2 & 2 & 1 \end{pmatrix},$$

$$X_{13}^{(1)c} = \begin{pmatrix} 1 & -2 & -1 & -1 & 4 & 1 & 1 & 2 & 2 & 1 \\ 1 & -2 & 0 & 1 & 4 & 0 & 1 & 0 & -2 & 0 \\ 1 & -2 & 1 & -1 & 4 & 1 & 1 & -2 & 2 & -1 \\ 1 & -2 & 1 & 1 & 4 & 1 & 1 & -2 & -2 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 0 & 1 & 1 & 0 & 1 & 0 & -1 & 0 \\ 1 & 1 & 0 & -1 & 1 & 0 & 1 & 0 & -1 & 0 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & -1 & 4 & 0 & 1 & 0 & -2 & 0 \end{pmatrix}.$$

The information matrix and its determinant are as follows:

$$M\left\{\xi_{13}^{(1)}\right\} = \begin{pmatrix} 13 & 6 & -1 & 1 & 34 & 9 & 13 & -2 & 4 & -1 \\ 6 & 34 & -2 & 4 & 24 & 6 & 6 & -4 & 4 & 2 \\ -1 & -2 & 9 & -1 & -4 & -1 & -1 & 6 & 2 & 1 \\ 1 & 4 & -1 & 13 & -4 & 1 & 1 & 2 & 6 & -1 \\ 34 & 24 & -4 & 4 & 118 & 24 & 34 & 4 & 10 & -4 \\ 9 & 6 & -1 & 1 & 24 & 9 & 9 & -2 & -2 & -1 \\ 13 & 6 & -1 & 1 & 34 & 9 & 13 & -2 & 4 & -1 \\ -2 & -4 & 6 & 2 & 4 & -2 & -2 & 24 & -4 & -2 \\ 4 & 4 & 2 & 6 & 10 & -2 & 4 & -4 & 34 & -2 \\ -1 & 2 & 1 & -1 & -4 & -1 & -1 & -2 & -2 & 9 \end{pmatrix},$$

$$\text{Det}\left\{M\left(\xi_{13}^{(1)}\right)\right\} = 0.$$

The 10×10 information matrix, $M(\xi_{13}^{(1)})$, has a zero determinant and is therefore singular and non-invertible. The variances of the predicted response, $\mathbf{x}_i' M^{-1}\{\xi_{13}^{(1)}\}\mathbf{x}_i$, can only be evaluated using the Penrose inverse of $M(\xi_{13}^{(1)})$ through singular value decomposition (SVD).

MATLAB 7.5.0 (R200b) provides the singular value decomposition of $M(\xi_{13}^{(1)})$ as:

$$\text{svd}\left\{M\left(\xi_{13}^{(1)}\right)\right\} = \begin{pmatrix} 151.4177 \\ 38.6717 \\ 30.1252 \\ 24.4260 \\ 12.7040 \\ 7.6777 \\ 6.2330 \\ 3.5060 \\ 1.2388 \\ 0.0000 \end{pmatrix},$$

where $[U, \Sigma, V] = \text{svd}\left\{M\left(\xi_{13}^{(1)}\right)\right\}$ gives:

$$U = \begin{pmatrix} -0.265 & 0.005 & -0.024 & 0.174 & 0.001 & -0.349 & -0.019 & -0.396 & 0.347 & -0.707 \\ -0.220 & -0.336 & 0.676 & -0.578 & 0.127 & -0.007 & -0.134 & -0.106 & 0.039 & 0.000 \\ 0.032 & 0.014 & -0.220 & -0.215 & 0.367 & -0.628 & -0.287 & 0.536 & 0.079 & -0.000 \\ -0.042 & -0.177 & -0.079 & -0.250 & -0.821 & -0.268 & 0.274 & 0.250 & 0.125 & -0.000 \\ -0.874 & 0.152 & -0.130 & 0.025 & 0.036 & 0.284 & 0.038 & 0.336 & -0.020 & -0.000 \\ -0.189 & 0.090 & 0.122 & 0.104 & -0.050 & -0.435 & 0.131 & -0.183 & -0.830 & 0.000 \\ -0.265 & 0.005 & -0.02 & 00.174 & 0.001 & -0.349 & -0.019 & -0.396 & 0.347 & 0.707 \\ -0.006 & 0.351 & -0.472 & -0.696 & 0.064 & 0.070 & 0.092 & -0.385 & -0.058 & 0.000 \\ -0.0970 & -0.806 & -0.482 & 0.012 & 0.048 & 0.102 & -0.193 & -0.156 & -0.187 & 0.000 \\ -0.023 & 0.227 & 0.014 & 0.014 & -0.408 & 0.071 & -0.872 & -0.083 & -0.098 & 0.000 \end{pmatrix},$$

$$\Sigma = \begin{pmatrix} 151.418 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 038.672 & & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 30.125 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 24.426 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.704 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7.678 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6.233 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.506 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.239 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 \end{pmatrix},$$

$$V = \begin{pmatrix} -0.265 & 0.005 & -0.024 & 0.174 & 0.001 & -0.349 & -0.020 & -0.396 & 0.347 & -0.707 \\ -0.220 & -0.336 & 0.676 & -0.578 & 0.127 & -0.007 & -0.134 & -0.106 & 0.039 & 0.000 \\ 0.034 & 0.014 & -0.220 & -0.218 & 0.367 & -0.628 & -0.287 & 0.536 & 0.079 & 0.000 \\ -0.042 & -0.177 & -0.079 & -0.250 & -0.821 & -0.268 & 0.278 & 0.250 & 0.125 & 0.000 \\ -0.874 & 0.152 & -0.130 & 0.025 & 0.036 & 0.284 & 0.038 & 0.336 & -0.020 & -0.000 \\ -0.189 & 0.090 & 0.122 & 0.104 & -0.050 & -0.435 & 0.131 & -0.183 & -0.830 & -0.000 \\ -0.265 & 0.005 & -0.024 & 0.174 & 0.001 & -0.349 & -0.019 & -0.396 & 0.347 & 0.707 \\ -0.006 & 0.351 & -0.472 & -0.696 & 0.064 & 0.070 & 0.092 & -0.385 & -0.058 & 0.000 \\ -0.097 & -0.806 & -0.482 & 0.012 & 0.048 & 0.102 & -0.193 & -0.156 & -0.187 & -0.000 \\ -0.023 & 0.227 & 0.014 & 0.014 & -0.408 & 0.071 & -0.872 & -0.083 & -0.098 & -0.000 \end{pmatrix}.$$

From these results, it is also established that:

(i) $M\left(\xi_{12}^{(1)}\right) = U\mathbf{\Sigma}V'$,

(ii) The Penrose inverse of $(X'X)$ is $(X'X)^+ = V\mathbf{\Sigma}^{-1}U'$.

The variances evaluated from $\mathbf{x}_i'\,(X'X)^+\,\mathbf{x}_i$ are shown in Table 3.2.

3.3 Discussion of results

This study addressed the problem caused by the effect of a singular information matrix in the initial designs of the quadratic portions for a three-variable response function within a variance exchange process. The results of the analysis, based on data generated from designs of sizes 12 and 13, are summarized in Tables 3.1 and 3.2, respectively. These tables present the variances of the predicted responses at different variance points, demonstrating that the information matrices of both initial designs, upon applying the Moore-Penrose inverse, are invertible.

Furthermore, the minimum variance of the initial designs is less than the maximum variance of the corresponding complement designs, as shown by the following relationships:

$$\max_{\mathbf{x}\in X_{12}^{(1)c}} d\left(\mathbf{x}_w, \xi_{12}^{(1)}\right) = 7.8704 > \min_{\mathbf{x}\in X_{12}^{(1)}} d\left(\mathbf{x}_v, \xi_{12}^{(1)}\right) = 0.4440,$$

$$\max_{\mathbf{x}\in X_{13}^{(1)c}} d\left(\mathbf{x}_w, \xi_{13}^{(1)}\right) = 2.4771 > \min_{\mathbf{x}\in X_{13}^{(1)}} d\left(\mathbf{x}_v, \xi_{13}^{(1)}\right) = 0.4367.$$

These differences in optimum variances demonstrate that variance exchange is feasible. Specifically, minimum variance points in the designs can be exchanged with maximum variance points from the complement designs.

Table 3.2: Variances of points for the initial two-variable linear 13-point designs

Vector	Current Design		Complement Design	
	Vector Point	Var	Vector Point	Var
$\mathbf{x}_1$	$(1 -2 -1\ 1\ 4\ 1\ 1\ 2 -1 -1)$	0.9119	$(1 -2 -1 -1\ 4\ 1\ 1\ 2\ 2\ 1)$	2.2958
$\mathbf{x}_2$	$(1 -2\ 0 -1\ 4\ 0\ 1\ 0\ 2\ 0)$	0.6858	$(1 -2\ 0\ 1\ 4\ 0\ 1\ 0 -2\ 1)$	2.0010
$\mathbf{x}_3$	$(1 -1\ 0 -1\ 1\ 0\ 1\ 0\ 1\ 0)$	0.4367	$(1 -2\ 1 -1\ 4\ 1\ 1 -2\ 2 -1)$	1.6021
$\mathbf{x}_4$	$(1 -1\ 1 -1\ 1\ 1\ 1 -1\ 1 -1)$	0.6174	$(1 -2\ 1\ 1\ 4\ 1\ 1 -2 -2\ 1)$	2.4771
$\mathbf{x}_5$	$(1 -1\ 1\ 1\ 1\ 1\ 1 -1 -1\ 1)$	0.8551	$(1 -1 -1 -1\ 1\ 1\ 1\ 1\ 1\ 1)$	1.7240
$\mathbf{x}_6$	$(1\ 1 -1 -1\ 1\ 1\ 1 -1 -1\ 1)$	0.6464	$(1 -1 -1\ 1\ 1\ 1\ 1\ 1 -1 -1)$	1.0821
$\mathbf{x}_7$	$(1\ 1 -1\ 1\ 1\ 1\ 1 -1\ 1 -1)$	0.5417	$(1 -1\ 0\ 1\ 1\ 0\ 1\ 0 -1\ 0)$	1.0007
$\mathbf{x}_8$	$(1\ 1\ 0\ 1\ 1\ 0\ 1\ 0\ 1\ 0)$	0.7317	$(1\ 1\ 0 -1\ 1\ 0\ 1\ 0 -1\ 0)$	0.7600
$\mathbf{x}_9$	$(1\ 2 -1 -1\ 4\ 1\ 1 -2 -2\ 1)$	0.6468	$(1\ 1\ 1 -1\ 1\ 1\ 1\ 1 -1 -1)$	0.7032
$\mathbf{x}_{10}$	$(1\ 2 -1\ 1\ 4\ 1\ 1\ 1 -2\ 2 -1)$	0.6468	$(1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1\ 1)$	0.7417
$\mathbf{x}_{11}$	$(1\ 2\ 0\ 1\ 4\ 0\ 1\ 0\ 2\ 0)$	0.4898	$(1\ 2\ 0 -1\ 4\ 0\ 1\ 0 -2\ 0)$	1.2063
$\mathbf{x}_{12}$	$(1\ 2\ 1 -1\ 4\ 1\ 1\ 1\ 2 -2 -1)$	0.9308		
$\mathbf{x}_{12}$	$(1\ 2\ 1\ 1\ 4\ 1\ 1\ 2\ 2\ 1)$	0.9400		

4 Conclusion

This work investigated a technique for overcoming the challenges of variance exchange processes when quadratic component designs of three-variable response polynomial functions are involved. At the initial stages of such designs, the determinants of the information matrices are typically zero, rendering the matrices non-invertible. Consequently, variances of predicted responses at different design points, which are necessary for variance exchanges, cannot be determined.

The results obtained show that the proposed algorithm successfully overcame these challenges. By applying the algorithm, the zero-determinant matrices were inverted, the variances of the predicted responses were evaluated, and the variance exchange process became possible.

It is concluded, therefore, that when the starting design of a quadratic three-variable design is singular, the constructed algorithm should be applied to evaluate the variances of the predicted responses at the design points and facilitate the variance exchange process.

Declarations

Availability of data and materials

The work utilized only generated data from the experimental space of the three-variable response model. Data sharing is not applicable to this article.

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Authors' contributions

Both authors collaborated on this work. They both read and approved the final manuscript.

Conflict of interest

The authors declare that they have no conflicts of interest related to this work.

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