CONDITIONS FOR OPTIMALITY AND VALIDITY OF SIMPLE LEAST SQUARES THEORY

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1. Notation and introduction. A matrix is denoted by a bold face letter such as A, X, Σ etc. For a matrix X of order n \times m
R(X) represents the rank of X.
\text{Null}(X) represents the linear space generated by the columns of X.
X^- represents a g-inverse as defined by Rao (1962, 1966, 1967b).
P_x = X(X'X)^{-1}X' is the projection operator which projects arbitrary n-vectors onto \text{Null}(X).
X^+ denotes a matrix of maximum rank such that X'X^+ = 0.
I denotes an identity matrix. The order of I will usually not be explicitly mentioned but can always be determined from the context.

Consider the Gauss-Markoff model (Y, X\beta, Σ) where Y is a vector of observations, E(Y) = X\beta and D(Y) = Σ, X being a given matrix of order n \times m and \beta a vector of unknown parameters. In the context of the discussion of the present paper, the model will be simply referred to as (X, Σ). The best linear unbiased estimator (BLUE) of an estimable parametric function p'\beta, where p is a vector, under the model (X, Σ) is a linear function L'Y such that E(L'Y) = p'\beta and L'ΣL is a minimum. It is well known that a BLUE under (X, Σ) can be obtained by the general method of least squares (see Rao, 1965, page 188 and Mitra and Rao, 1968).

The BLUE of p'\beta under (X_0, Σ_0) is said to be (X, Σ) optimal if it is also the BLUE of p'\beta under the model (X, Σ). The object of the present paper is to characterize the set of (X, Σ) such that for every estimable parametric function the BLUE under a given model (X_0, σ^2I) is (X, Σ)-optimal. Further, the classes of Σ for which different statistical methods based on (X, σ^2I) remain valid have been obtained.

In previous papers Rao (1967a, 1968)\(^1\) gave the necessary and sufficient conditions for BLUE under (X, Σ_0) to be (X, Σ)-optimal, in which case the investigation was confined to the characterization of Σ only. Similar results, but not providing an exact representation of Σ, were also obtained by Zyskind (1967), Watson (1967) and Kruskal (1968) in the special case of Σ_0 = σ^2I.

2. The main results.

Lemma 2.1. If for every estimable parametric function the BLUE under (X_0, σ^2I) is (X, σ^2I)-optimal, it is necessary and sufficient that X is of the form

\begin{equation}
X = X_0 + (I - P_{x_0})A,
\end{equation}

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\(^1\) The results were first given in a lecture at the Fifth Berkeley Symposium in 1965.
where \( A \) is any matrix such that

\[
(2.2) \quad \mathcal{M}(A') \cap \mathcal{M}(X_0') = \{0\},
\]

a set consisting exclusively of the null vector, or equivalently

\[
(2.3) \quad X = X_0 + (I - P_{x_0})F[I + (I - P_{x_0'})D]^{+'},
\]

where \( D \) and \( F \) are arbitrary.

We note that from standard results in the Gauss-Markoff theory (see Rao, 1965, page 178) it suffices to investigate conditions under which the elements of the vector \( X_0'Y \) have the same expectations and minimum variance under the models \( (X_0, \sigma^2 I) \) and \( (X, \sigma^2 I) \).

**Sufficiency of (2.1) and (2.2).** Let \( X \) be of the form given in (2.1) and (2.2). Then

\[
E(X_0'Y | X, \sigma^2 I) = X_0'X0 = E(X_0'Y | X_0, \sigma^2 I),
\]

since \( I - P_{x_0} \) is symmetric and \( (I - P_{x_0})X_0 = 0 \).

Let \( Z = X_0' \), in which case \( X'Z = 0 \). By definition \( X_0'Z + A'(I - P_{x_0})Z \), i.e., \( X_0'Z = -A'(I - P_{x_0})Z \), which is a contradiction in view of (2.2) unless \( X_0'Z = 0 \). Hence by Lemma (i), page 257 in Rao, 1965, sufficiency is established.

**Necessity of (2.1) and (2.2).** Let a BLUE under \( (X_0, \sigma^2 I) \) be \( (X, \sigma^2 I) \) optimal. Necessity of (2.1) is obvious for expectations of \( X_0'Y \) to be the same under the two models. Now suppose that \( \mathcal{M}(A'(I - P_{x_0})) \cap \mathcal{M}(X_0') \) contains a vector \( \alpha \neq 0 \), in which case \( \alpha = A'(I - P_{x_0})y = X_0'X0 \lambda \) for some vectors \( y \) and \( \lambda \). Let \( z = X_0'X0 \lambda - (I - P_{x_0})y. \) Check that \( X_0'Z = 0 \) and observe that \( X_0'Z = X_0'X0 \lambda = \alpha \neq 0 \). This shows that at least some elements of \( X_0'Y \) are correlated with \( z'Y \) which is a contradiction. Hence \( \mathcal{M}(A'(I - P_{x_0})) \cap \mathcal{M}(X_0') = \{0\} \). Necessity of (2.2) follows from the fact that, without loss of generality, one may take \( A \) to be \( (I - P_{x_0})A \).

**Necessity and sufficiency of (2.3).** Using the condition of unbiasedness

\[
E(X_0'Y | X_0, \sigma^2 I) = E(X_0'Y | X, \sigma^2 I) \Rightarrow X = X_0 + (I - P_{x_0})G.
\]

Let \( Z = X^+ \) and \( C \) stand for covariance. Since \( X_0'Y \) are BLUE's under \( (X, \sigma^2 I) \),

\[
C(Z', X_0'Y | X, \sigma^2 I) = 0 \Rightarrow X_0 = XH \quad \text{for some } H.
\]

Multiplying both sides of \( X = X_0 + X_0^+G \) by \( H \) and writing \( X_0 = XH \) we obtain

\[
X_0 = X_0H + X_0^+GH \Rightarrow X_0 = X_0H \quad \text{and} \quad GH = 0.
\]

Observe that \( X_0 = X_0H \Rightarrow H = I + (I - P_{x_0'})D \) for some \( D \) and since \( GH = 0 \),

\[
G = F(H^+) = F[I + (I - P_{x_0'})D]^{+'}.
\]

Hence

\[
X = X_0 + (I - P_{x_0})F[I + (I - P_{x_0'})D]^{+'},
\]

where \( F \) and \( D \) are arbitrary.
COROLLARY 1. A sufficient condition that for every estimable function the BLUE under \((X_0, \sigma^2)\) is \((X, \sigma^2)\)-optimal is

\[(2.4) \quad X = X_0 + [I - X_0 (X_0'X_0)^{-1}X_0']B[I - X_0'X_0(X_0'X)^{-1}],\]

where \(B\) is arbitrary.

COROLLARY 2. If \(R(X_0)\) is equal to the number of columns in \(X_0\), then the conditions of Lemma 2.1 reduce to \(X = X_0\).

PROOF.

\[(2.5) \quad E(X_0'Y | X, \sigma^2) = X_0'X_0\beta \Rightarrow X = X_0 + X_0'G,\]

for some \(G\). Since \(X_0'Y\) are BLUE's under \((X, \sigma^2)\),

\[(2.6) \quad C(X_0', Y' | X, \Sigma) = 0 \Rightarrow X_0'Z = 0 \Rightarrow X_0 = XD,\]

for some \(D\). From (2.5) and (2.6),

\[XD = X_0D + X_0'GD = X_0.\]

Multiplying by \(X_0'\),

\[X_0'X_0 = X_0'X_0D \Rightarrow D = I,

since \(X_0'X_0\) is non-singular. Then \(X_0 = X\) from (2.6).

LEMMA 2.2. For the BLUE under \((X_0, \sigma^2)\) to be \((X, \Sigma)\)-optimal for every estimable parametric function, it is necessary and sufficient that

\[(2.7) \quad X = X_0 + Z_0G,

(2.8) \quad \Sigma = X_0AX_0' + Z_0BZ_0' + X_0A'G'Z_0' + Z_0GAX_0',

where \(A, B, G\) are arbitrary except that \(\Sigma\) is non-negative definite and \(Z_0\) is written for \(X_0\).

PROOF OF Necessity. As in Lemma 2.1, we consider the functions \(X_0'Y\). The condition that \(E(X_0'Y)\) is the same for \((X_0, \sigma^2)\) and \((X, \Sigma)\) implies that

\[(2.9) \quad X = X_0 + Z_0G,

for some \(G\). If \(X_0'Y\) is optimal for \((X, \Sigma)\), then

\[C(X_0', Y' | X, \Sigma) = X_0'\Sigma Z = 0,

where \(Z = X^+.\) We write

\[(2.10) \quad \Sigma = X_0\Sigma_1X_0' + Z_0\Sigma_2Z_0' + X_0\Sigma_3Z_0' + Z_0\Sigma_4X_0',

where \(\Sigma_1\) and \(\Sigma_2\) are symmetrical, as in Rao (1968, equation 2.8). Then

\[X_0'\Sigma Z = X_0'(X_0\Sigma_1X_0' + X_0\Sigma_2Z_0')Z = 0 \Rightarrow X_0\Sigma_1X_0'X_0 = X_0\Sigma_2X_0'\]

\[= XM = X_0M + Z_0GM \Rightarrow X_0\Sigma_1X_0'X_0 = X_0M, \quad X_0\Sigma_2X_0' = X_0M(X_0'X_0)^{-1}X_0',

\[Z_0\Sigma_3X_0'X_0 = Z_0GM, \quad Z_0\Sigma_4X_0' = Z_0GM(X_0'X_0)^{-1}X_0'.\]

Writing \(A = M(X_0'X_0)^{-1}, B = \Sigma_2, \Sigma\) can be written in the form (2.8).
Note 1. In Corollary 2 to Lemma 2.1, it was noted that \( \mathbf{X} = \mathbf{X}_0 \) when the rank of \( \mathbf{X}_0 \) is full and \( \Sigma \) is restricted to the form \( \sigma^2 \mathbf{I} \). This result need not be true, when a general \( \Sigma \), as in (2.10), is considered.

Note 2. Lemma 2.2 asserts that, when \( \mathbf{X} \) and \( \Sigma \) are as in (2.7, 2.8), a BLUE of an estimable parametric function under \( (\mathbf{X}_0, \sigma^2 \mathbf{I}) \) is also a BLUE under \( (\mathbf{X}, \Sigma) \). But this does not imply that the minimum variances attained in the two models are the same. To compare the variances let us first compute the dispersion matrices of \( \mathbf{X}_0' \mathbf{Y} \) under the two models.

\[
D(\mathbf{X}_0' \mathbf{Y} \mid \mathbf{X}_0, \sigma^2 \mathbf{I}) = \sigma^2 \mathbf{X}_0' \mathbf{X}_0,
\]

\[
D(\mathbf{X}_0' \mathbf{Y} \mid \mathbf{X}, \Sigma \text{ as in 2.8}) = \mathbf{X}_0' \mathbf{X}_0 \mathbf{A} \mathbf{X}_0' \mathbf{X}_0.
\]

If the variances of a BLUE are to be equal, a necessary and sufficient condition is

\[
(2.11) \quad \sigma^2 \mathbf{X}_0' \mathbf{X}_0 = \mathbf{X}_0' \mathbf{X}_0 \mathbf{A} \mathbf{X}_0' \mathbf{X}_0,
\]

or \( \mathbf{A} = \sigma^2 (\mathbf{X}_0' \mathbf{X}_0)^{-} \), while \( \mathbf{B} \) and \( \mathbf{G} \) in (2.8) can be arbitrary.

**Lemma 2.3.** Let \( \mathbf{P} \) be a matrix of order \( m \times k \) such that \( \mathbb{M}(\mathbf{P}) \subset \mathbb{M}(\mathbf{X}_0') \) and \( R(\mathbf{P}) = k \). A necessary and sufficient condition for \( \mathbf{L}' \mathbf{Y} = \mathbf{P}' (\mathbf{X}_0' \mathbf{X}_0) \mathbf{X}_0' \mathbf{Y} \) to be the BLUEs for \( \mathbf{P}' \mathbf{G} \) under \( (\mathbf{X}, \sigma^2 \mathbf{I}) \) is that

\[
(2.12) \quad \mathbf{X} = \mathbf{X}_0 + [\mathbf{I} - (\mathbf{L}' \mathbf{L})'] [\mathbf{C} \mathbf{B}^{-} + \mathbf{D} (\mathbf{I} - \mathbf{B} \mathbf{B}^{-})],
\]

where \( \mathbf{B} = (\mathbf{P}' \mathbf{L})' \mathbf{L} \), \( \mathbf{C} = \mathbf{L} - \mathbf{X}_0 \mathbf{B} \) and \( \mathbf{D} \) an arbitrary matrix of order \( n \times m \).

**Proof of Sufficiency.** The sufficiency part follows from the fact that \( \mathbf{L}' \mathbf{X} = \mathbf{L}' \mathbf{X}_0 = \mathbf{P}' \) and \( \mathbf{X} \mathbf{B} = \mathbf{X}_0 \mathbf{B} + [\mathbf{I} - (\mathbf{L}' \mathbf{L})'] \mathbf{C} = \mathbf{X}_0 \mathbf{B} + \mathbf{C} = \mathbf{L} \) since \( R(\mathbf{P}) = k \Rightarrow R(\mathbf{L}) = k \Rightarrow R(\mathbf{B}) = k \Rightarrow \mathbf{B}^{-} \mathbf{B} = \mathbf{I} \), and \( \mathbf{L}' \mathbf{C} = \mathbf{L}' \mathbf{L} - \mathbf{X}_0 \mathbf{B} = \mathbf{L}' \mathbf{L} - \mathbf{P}' \mathbf{B} = \mathbf{0} \).

**Proof of Necessity.** To establish the necessity part note that

\[
E(\mathbf{L}' \mathbf{Y} | \mathbf{Y}, \Sigma, \sigma^2 \mathbf{I}) = \mathbf{P}' \mathbf{G} = \mathbf{L}' (\mathbf{X} - \mathbf{X}_0) = 0 \Rightarrow \mathbf{X} = \mathbf{X}_0 + [\mathbf{I} - (\mathbf{L}' \mathbf{L})'] \mathbf{G}.
\]

Further, the fact that \( \mathbf{L}' \mathbf{Y} \) is BLUE for \( \mathbf{P}' \mathbf{G} \) under \( (\mathbf{Y}, \Sigma, \sigma^2 \mathbf{I}) \) \( \Rightarrow \mathbf{L} = \mathbf{X} \mathbf{B} \) for some \( \mathbf{B} \Rightarrow \mathbf{L}' \mathbf{L} = \mathbf{L}' \mathbf{X} \mathbf{B} = \mathbf{P}' \mathbf{B} \Rightarrow \mathbf{B} = (\mathbf{P}' \mathbf{L})' \mathbf{L} \). The rest of the lemma follows from the general solution (G) of the equation \( \mathbf{A} \mathbf{G} \mathbf{B} = \mathbf{C} \), given in Theorem 2d of Rao (1967b) substituting \( \mathbf{A} = \mathbf{I} - (\mathbf{L} \mathbf{L})' \).

**Lemma 2.4.** Let us consider two alternative models \( (\mathbf{X}, \sigma^2 \mathbf{I}) \) and \( (\mathbf{X}, \Sigma) \) where \( \Sigma \) has the general representation \( \Sigma = \mathbf{X} \Sigma_0 \mathbf{X}' + \mathbf{Z} \Sigma_0' \mathbf{Z}' + \mathbf{X} \Sigma_2' \mathbf{X}' \). Then the following are true.

(a) \( D(\mathbf{X}' \mathbf{Y} | \sigma^2 \mathbf{I}) = D(\mathbf{X}' \mathbf{Y} | \Sigma) \Rightarrow \Sigma_1 = \sigma^2 (\mathbf{X}' \mathbf{X})^- \).

(b) Let \( R_0^2 = \min_\mathbf{g} (\mathbf{Y} - \mathbf{X}_0 \mathbf{g})' (\mathbf{Y} - \mathbf{X}_0 \mathbf{g}) = \mathbf{Y}' (\mathbf{I} - \mathbf{P}_x) \mathbf{Y} \). Then
\[
E[\mathbf{Y}' (\mathbf{I} - \mathbf{P}_x) \mathbf{Y} | \sigma^2 \mathbf{I}] = E[\mathbf{Y}' (\mathbf{I} - \mathbf{P}_x) \mathbf{Y} | \Sigma] \Rightarrow \text{trace} \mathbf{Z} \Sigma_2' \mathbf{Z}' = (n - r) \sigma^2
\]
where \( r \) is the rank of \( \mathbf{X} \) and \( n \) is the number of elements in \( \mathbf{Y} \).

(c) Let \( \mathbf{Y} \) have a multivariate normal distribution. Then the distribution \( R_0^2 / \sigma^2 \) under \( (\mathbf{X}, \Sigma) \) is \( \chi^2 \) on \( (n - r) \) degrees of freedom iff \( (\mathbf{Z} \Sigma_2' \mathbf{Z}') / \sigma^2 = (\mathbf{I} - \mathbf{P}_x) \). If further \( \mathbf{X}' \mathbf{Y} \) and \( R_0^2 \) are to be independently distributed, then \( \mathbf{X} \Sigma_2' \mathbf{Z}' = \mathbf{Z} \Sigma_2' \mathbf{X}' = \mathbf{0} \).
Proof. The result (a) is easily established. To prove (b), we observe that

\[(2.13) \quad E [Y' (I - P_x) Y | \Sigma] = \text{trace} \left[ (I - P_x) \Sigma \right] \]
\[= \text{trace} \left( Z \Sigma \Sigma' + Z \Sigma \Sigma' \right) = \text{trace} Z \Sigma Z'. \]

Since \( E (Y' (I - P_x) Y / \sigma^2) = (n - r) \sigma^2 \), the result (b) is established.

The necessary and sufficient condition for \( Y' (I - P_x) Y / \sigma^2 \) to have a \( \chi^2 \)-distribution is (using the condition on page 443 of Rao, 1965)

\[ \Sigma (I - P_x) \Sigma (I - P_x) \Sigma = \sigma^2 \Sigma (I - P_x) \Sigma \]
\[\iff (Z \Sigma \Sigma' + X \Sigma \Sigma') (Z \Sigma \Sigma' + Z \Sigma X') \]
\[= \sigma^2 (Z \Sigma \Sigma' + X \Sigma \Sigma') (Z \Sigma \Sigma' + Z \Sigma X') \]
\[\iff Z' Z \Sigma \Sigma' Z \Sigma \Sigma' Z \Sigma \Sigma' = \sigma^2 Z \Sigma \Sigma' Z \Sigma \Sigma' Z \Sigma \Sigma' \]
\[\iff (Z \Sigma \Sigma') (Z \Sigma \Sigma') (Z \Sigma \Sigma') = \sigma^2 (Z \Sigma \Sigma') (Z \Sigma \Sigma') \]
\[\iff (Z \Sigma \Sigma') / \sigma^2 \text{ is idempotent.} \]

The df of \( \chi^2 \) is (see page 443 Rao, 1965)

\[(2.15) \quad \text{trace} (I - P_x) \Sigma / \sigma^2 = \text{trace} (Z \Sigma \Sigma' + Z \Sigma X') / \sigma^2 \]
\[= \text{trace} Z \Sigma Z' / \sigma^2. \]

If \( \text{trace} Z \Sigma Z' = (n - r) \sigma^2 \), then we should have

\[(2.16) \quad Z \Sigma Z' = \sigma^2 (I - P_x). \]

If \( Y' \) and \( Y' (I - P_x) Y \) are to be independently distributed, then \( X' \Sigma (I - P_x) = 0 \Rightarrow X \Sigma \Sigma' = Z \Sigma X' = 0 \). Thus (c) is proved.

The following table gives the necessary and sufficient conditions on \( \Sigma \) for different procedures in the simple least squares theory (i.e. assuming \( \Sigma = \sigma^2 I \)) to be optimal or valid.

<table>
<thead>
<tr>
<th>Property</th>
<th>Representation of ( \Sigma )</th>
</tr>
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<tbody>
<tr>
<td>(i) Every SLSE is BLUE</td>
<td>( X \Sigma X' + Z \Sigma Z' )</td>
</tr>
<tr>
<td>(ii) Expression for variance of a SLSE remains the same</td>
<td>( \sigma^2 P_x + Z \Sigma Z' + X \Sigma X' + Z \Sigma X' )</td>
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<tr>
<td>(iii) ( R_o / \sigma^2 ) is a ( \chi^2 ) on ( (n - r) ) df</td>
<td>( X \Sigma X' + \sigma^2 (I - P_x) + X \Sigma Z' + Z \Sigma X' )</td>
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<tr>
<td>(iv) Every SLSE and ( R_o ) are independently distributed</td>
<td>( X \Sigma X' + Z \Sigma Z' )</td>
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<tr>
<td>(v) In addition to (iv), ( R_o / \sigma^2 ) is a ( \chi^2 ) on ( (n - r) ) df</td>
<td>( X \Sigma X' + \sigma^2 (I - P_x) )</td>
</tr>
<tr>
<td>(vi) In addition to (v), (ii) is satisfied</td>
<td>( \sigma^2 I )</td>
</tr>
<tr>
<td>(vii) In addition to (v), the variance of a particular SLSE, say that of ( p \bar{p} ) is the same</td>
<td>( \sigma^2 I + XAX' ) where ( p'Ap = 0 )</td>
</tr>
</tbody>
</table>
From the table we observe that while some of the procedures based on simple least squares theory are valid for a wider class of $\Sigma$, for the full battery of procedures on estimation and testing to be applicable (case vi), it is necessary that $\Sigma = \sigma^2 I$. Case (vii) shows that if the procedures are to be valid for particular parametric functions, then $\Sigma$ can belong to a wider class. A well known example which falls in this category is the treatment of two way classification (mixed model) discussed in Rao (1965, page 216).

3. Tests of linear hypotheses when (2.1) holds. Consider a parametric function $p'\beta$ which is estimable under the model $(Y, X_0\beta, \sigma^2 I)$. It is clear that if the true model $(Y, X\beta, \sigma^2 I)$ satisfies the conditions of Lemma 2.1, the expression for the BLUE of $p'\beta$ and for its variance as well remain unchanged in either case. Notice, however, that if $R_0^2$ denotes the residual sum of squares obtained under $(Y, X_0\beta, \sigma^2 I)$

$$E[R_0^2 | X_0\beta, \sigma^2 I] = E[tr Y'(I - P_{X_0})Y | X_0\beta, \sigma^2 I]$$
$$= E[tr (I - P_{X_0})YY' | X_0\beta, \sigma^2 I]$$
$$= tr (I - P_{X_0})(\sigma^2 I + X_0\beta'X')$$
$$= (n - r)\sigma^2 + \beta'X'(I - P_{X_0})X\beta$$
$$= (n - r)\sigma^2 + \beta'A'(I - P_{X_0})A\beta$$

which is equal to $(n - r)\sigma^2$ if and only if $(I - P_{X_0})A\beta = 0$ that is $X_0\beta = X_0\beta$.

This shows that if the two models are distinct (a) $R_0^2/(n - r)$ overestimates $\sigma^2$ and (b) $R_0^2/\sigma^2$ is distributed as noncentral chi-square on $(n - r)$ df, with the noncentrality parameter $\lambda = \beta'A'(I - P_{X_0})A\beta/\sigma^2$, independently of the BLUE $p'\beta$. Hence

$$(p'\hat{\beta} - p'\beta)/(p'(X_0'X_0)^{-1}pR_0^2/(n - r))^\frac{1}{2}$$

is distributed as the ratio of a standard normal variable and an independent root mean (noncentral) chi-square on $(n - r)$ df. Also the usual $F$-statistic, computed for testing several linear hypotheses on unknown parameters, is, in the null case, distributed as the ratio of a (central) mean chi-square and an independent mean (noncentral) chi-square on $(n - r)$ df. For various values of the noncentrality parameter $\lambda$, the following table gives the true level attained by the $F$-test under the model $(X, \sigma^2 I)$ when 1 per cent and 5 per cent critical values under the model $(X_0, \sigma^2 I)$ are used.

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\( \alpha = 5\% \), \( n_2 = 30 \)

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\( \alpha = 5\% \), \( n_2 = 40 \)

REFERENCES


