Optimal balanced measurement designs when errors are correlated


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Abstract

We consider measurement experiments in which unknown specimens as well as known standards are measured sequentially in time. The observations on standards are used to make appropriate adjustments to the observations on the unknown specimens. When measurement errors are correlated, the order of the measurements of the standards and the unknown specimens can have a significant effect on the precision of the estimated values for the unknowns. In this paper we consider measurement processes in which there is a constant unknown bias and the measurement errors follow an autoregressive process of order one. There are $n$ unknown specimens that need to be measured and a known standard is available for assessing the nature of the measurement errors. This paper considers the problem of determining a measurement design using which the unknown specimens can be measured with maximum average precision for a fixed cost. Optimum measurement designs are derived within the class of balanced designs. An algorithm for construction of balanced measurement designs is described.

Keywords: Calibration problems, systematic errors, random errors, maximum likelihood estimators, A-optimality, autoregressive processes.

1 Introduction

A measurement process is frequently subject to errors which are generally classified as systematic, or random, or a combination of both. The random errors are defined to have a zero expected value, and the systematic errors are defined to be due to biases in the measurement process. Thus, the measured (observed) value of an unknown specimen can be described by the following additive model.

\[ y_i = \mu_i + \tau_i + \epsilon_i \]  

(1.1)

where $\mu_i$, $\tau_i$ and $\epsilon_i$ denote the systematic error, the true value, and the random error, respectively, corresponding to the specimen being measured. If the errors can be estimated sufficiently precisely, then it may be possible to process the raw measurement to produce an estimate of the true value which is "better" than the raw observation itself.

Since "standards" have known true values, the errors associated with the measurement process are "observed" whenever a standard is measured. Typically, random errors are assumed to be independent, but it is often more realistic to acknowledge that the measurement process is serially correlated. For example, consider an automated system which measures the concentrations of a toxic material in water samples contained in each of several test tubes. These measurements are made sequentially in time. If the time period
between these measurements is relatively small, then it is quite conceivable that a substantial correlation may exist between consecutive random errors. Suppose the correlation structure can be modeled sufficiently well so that it may be assumed known. Then a measurement experiment consisting of several observations of each of \( m \) different unknown specimens and of a known standard may utilize the "known" correlation structure to give better estimates of the unknowns. The following example is used to illustrate how this occurs.

**Example 1.1:** Consider the simple situation where there are only random errors, i.e., the systematic errors are assumed to be zero. Let \( y_1 \) represent an observation of a standard and \( y_2 \) represent an observation of an unknown, and \( \tau_1 \) and \( \tau_2 \) represent the true values of the standard and the unknown, respectively. The relationship between the observed values and the true values may be written as

\[
\begin{bmatrix}
y_1 \\
y_2
\end{bmatrix}
= \begin{bmatrix}
\tau_1 \\
\tau_2
\end{bmatrix}
+ \begin{bmatrix}
\epsilon_1 \\
\epsilon_2
\end{bmatrix}
\]

Also suppose the random errors have the distribution

\[
\begin{bmatrix}
\epsilon_1 \\
\epsilon_2
\end{bmatrix}
\sim N\left(\begin{bmatrix}0 \\ 0\end{bmatrix}, \begin{bmatrix}1.0 & 0.9 \\ 0.9 & 1.0\end{bmatrix}\right)
\]

Since \( \epsilon_1 \) is observable, \( \epsilon_2 \) may be estimated by

\[
E(\epsilon_2 \mid \epsilon_1) = 0.9\epsilon_1
\]

Consequently, the unknown quantity may be estimated as

\[
\hat{\tau}_2 = y_2 - 0.9\epsilon_1
\]

The variance of this estimate is

\[
Var(\hat{\tau}_2) = 0.19
\]

which is less than 1, the variance of \( y_2 \).

The precision in estimating the true values of unknown specimens also depends on the arrangement (ordering) of the observations of the unknowns and the standard. The following example illustrates this phenomenon.

**Example 1.2:** Suppose a single measurement of one unknown is to be made along with two observations of the standard. The systematic errors are assumed to be zero, and the random errors of observations 1, 2, and 3 are normally distributed with mean zero and the covariance matrix

\[
\begin{bmatrix}
1.00 & 0.50 & 0.25 \\
0.50 & 1.00 & 0.50 \\
0.25 & 0.50 & 1.00
\end{bmatrix}
\]

If the observations are made in the order \( USS \) where \( U \) denotes the unknown specimen and \( S \) denotes the standard, then the unknown quantity may be estimated as

\[
\hat{\tau}_1 = y_1 - E(\epsilon_1 \mid \epsilon_2, \epsilon_3) = y_1 - 0.5\epsilon_2
\]

The variance of this estimate is

\[
Var(\hat{\tau}_1) = 0.75
\]

If the observations are made in the order \( SUS \), then the unknown quantity may be estimated as

\[
\hat{\tau}_2 = y_2 - E(\epsilon_2 \mid \epsilon_1, \epsilon_3) = y_2 - 0.4\epsilon_1 - 0.4\epsilon_3
\]
The variance of this estimate is

\[ \text{Var}(\hat{\tau}_S) = 0.00 \]

So the order SUS is preferable to the order USS.

Literature pertaining to calibration or measurement problems involving correlated errors appears to begin with Pepper (1973). He considered the following model for the measurement process.

\[ y_t = \tau + (b_t + \eta_t) \]

where \( y_t \) represents the measured value and \( \tau \) represents the corresponding true value, for \( t = 1, 2, \ldots, n \). The quantity \((b_t + \eta_t)\) represents random errors, where \( \eta_t \) are independent \( N(0, \sigma_\eta^2) \) random variables, and \( b_t \) arise from a random walk of the form

\[ b_t = b_{t-1} + \epsilon_t \]

with \( \epsilon_t \) independent \( N(0, \sigma_\epsilon^2) \) random variables which are also independent of \( \eta_t \). Pepper (1973) provided three different measurement policies. For each of the policies, he gave approximate maximum likelihood estimators (m.l.e.s) for the unknowns. In addition, he gave suggestions for ordering the observations based on enumeration of all possible designs in situations where the total number of observations is "small". Clearly, the computations required to carry out his plan become unfeasible as the number of observations grows.

The problem we address in this paper shares some similarities with various published results. For optimal block designs for estimating treatment differences when the errors are correlated, see Berenblut and Webb (1974), Cheng (1983, 1988), Ipinyomi (1986), Kiefer and Wynn (1981, 1983, 1984), Kunert (1985a, 1987), Martin (1982), Martin and Eccleton (1991), Russell and Eccleston (1987a, 1987b), and Williams (1985, 1986); for optimal repeated measurement designs for estimating all possible contrasts of the treatments, see Williams (1949), and Kunert (1985b); for optimal designs for the comparison of treatments to a control, see Hedayat, Jacroux and Majumdar (1988), Pigeon and Raghavarao (1987) and Majumdar (1988). However, none of these directly address the problem under consideration.

In the next section we describe our problem in detail and introduce some relevant terminology. Section 3 provides optimal designs, within the class of "balanced" designs, when there are three or more unknowns to be measured. For situations where at most two unknowns are to be measured we can actually find optimal designs in the class of all designs but we do not present the results here. Instead the reader is referred to Taylor (1989). Section 4 presents an algorithm to generate the optimal balanced designs. Section 5 gives an example which illustrates how to find the best balanced design while satisfying certain cost constraints.

2 Preliminaries

The problem

The specific problem treated in this paper assumes that a total of \( N \) measurements can be made some of which may be measurements on a standard while the remaining measurements are of \( m \) different unknown specimens. The standard as well as each of the specimens may be measured more than once if so desired. The number of measurements of unknown specimen \( i \) denoted by \( t_i \), \( i = 1, 2, \ldots, m \), and the number of measurements of the standard is denoted by \( b - 1 \) (\( b > 1 \)). Furthermore these observations are made sequentially in time. The statistical model assumes a constant but unknown systematic error, say \( \mu \). Let \( \tau_0 \)
be the true value of the standard (which is, of course, known), and \( \delta_{ij} \) be the indicator function defined by

\[
\delta_{ij} = \begin{cases} 
1 & \text{if } j = 0 \text{ and observation } i \text{ is of the standard} \\
1 & \text{if } j \in \{1, 2, \ldots, m\} \text{ and observation } i \text{ is of unknown } j \\
0 & \text{otherwise}
\end{cases}
\]

Then, the model described in (1.1) can be rewritten as

\[
y_i = \mu + \delta_{i0} \tau_0 + \sum_{j=1}^m \delta_{ij} \tau_j + \varepsilon_i \quad i = 1, \ldots, N
\]

(2.1)

The random errors \( \varepsilon_i \) are now assumed to arise from a first order autoregressive process (AR(1)) of the form

\[
\varepsilon_i = \phi \varepsilon_{i-1} + z_i
\]

(2.2)

where \( z_i \) are assumed to be independent \( N(0, \sigma^2) \) random variables, and the coefficient \( \phi \) (\(-1 < \phi < 1\)) is assumed known.

This paper is concerned with finding “balanced” measurement designs (to be defined shortly) using which the values corresponding to the unknown specimens can be estimated most efficiently. In particular, we consider the A-optimality criterion according to which the average variance of the maximum likelihood estimates of the true values of the unknown specimens is minimized. The following terminology is relevant to the rest of the paper.

**The class of “balanced measurement designs”**

A “Balanced Measurement Design” is defined here as a design for which the m.l.e.s of the true values of the unknown specimens have the same variance and all pairs of the estimators have the same covariance. Such a design is often desirable since inferences may be made without regard to the labelling of the specimens.

**Batches**

Designs used in this paper will be described in terms of “batches”. A “batch” is defined to be the set of all measurements of unknown specimens between two successive observations of the standard, or the set of all measurements (if any) of unknowns before the first measurement of a standard, or the set of all measurements (if any) of unknown specimens after the last measurement of a standard. A batch of measurements is called an “interior batch” if the corresponding measurements are sandwiched between measurements of the standard. If the batch of measurements forms the initial segment of the measurement process it is called the “initial batch” and if it forms the final segment of the measurement experiment, then it is called the “final batch”.

Empty batches are permissible and these occur when the standard is measured at two consecutive time points with no unknown in between. The number of empty batches is denoted by \( b_0 \). As a consequence of these definitions, \( b - 1 \) observations of a standard give rise to \( b \) batches. The following example is given to illustrate the above definitions.

**Example 2.1:** Consider the following sequence of the observations.

\[
U_1 U_2 SU_1 U_3 U_3 U_5 U_2 U_1 U_2 U_2 SS
\]

where \( U_i \) denotes the unknown specimen \( i \) and \( S \) denotes the standard. In this case, there are \( b = 4 \) batches. Of these 4 batches \( b_0 = 2 \) are empty. The initial batch consists of two measurements, the first being of
specimen 1 and the next of specimen 3. The first interior batch consists of the eight measurements in the order $U_1 U_2 U_3 U_2 U_1 U_2 U_2$. The second interior batch is empty since we have two successive measurements of the standard with no unknown specimen in between. The final batch is also empty since no unknowns are measured after the last measurement of the standard. Note that specimen 1 is measured $t_1 = 3$ times, specimen 2 is measured $t_2 = 3$ times, and specimen 3 is measured $t_3 = 4$ times. The total number of measurements is $N = (b - 1) + t_1 + t_2 + t_3 = 13$.

Maximum likelihood estimators for the unknown true values

Since $\tau_0$ is known in the model described in (2.1), we let

$$y_i^* = \begin{cases} y_i & \text{if observation } i \text{ is of the unknown} \\ y_i - \tau_0 & \text{if observation } i \text{ is of the standard} \end{cases}$$

Thus, we may write

$$y_i^* = \mu + \sum_{j=1}^{m} \delta_{i,j} \tau_j + \epsilon_i$$

or in matrix notation, this can be represented as

$$y^* = X\beta + \epsilon$$

where $X$ is $n \times (1 + m)$ defined as

$$X_{i,j} = \begin{cases} 1 & \text{if } j = 1 \\ \delta_{i,j} & \text{if } j > 1 \end{cases}$$

and $\beta = [\mu, \tau]'$ where $\tau = [\tau_1, \tau_2, \ldots, \tau_m]$. We write $X = [X_1, X_2]$ where $X_1$ is a column of 1’s and $X_2$ has $\delta_{i,j}$ as its $(i,j)$-element.

The random errors $\epsilon_i$ are assumed to arise from an AR(1) process described in (2.2). Hence, the vector of these random errors $\epsilon = [\epsilon_1, \epsilon_2, \ldots, \epsilon_N]$ has a multivariate normal distribution with a zero mean and a variance-covariance matrix $\sigma^2 V$, where $V$ is a positive definite matrix with the elements

$$V_{i,j} = \frac{\phi| i - j |}{1 - \phi^2}$$

It is well known (see Siddiqui (1958)) that $V^{-1}$ is given by

$$(V^{-1})_{i,j} = \begin{cases} 1 & \text{if } i = j = 1 \text{ or } i = j = N \\ 1 + \phi^2 & \text{if } i = j \text{ and } 1 < j < N \\ -\phi & \text{if } |i - j| = 1 \\ 0 & \text{otherwise} \end{cases}$$

The m.l.e. of $\beta$ is

$$\hat{\beta} = [\hat{\mu}, \hat{\tau}]' = (X'V^{-1}X)^{-1}X'V^{-1}y^*$$

and its variance is

$$Var(\hat{\beta}) = \sigma^2 (X'V^{-1}X)^{-1}$$

From this it is easy to see that the m.l.e. of $\tau$ is given by

$$\hat{\tau} = C^{-1}X_2'V^{-1} - V^{-1}X_1(X'V^{-1}X_1)^{-1}X_1'V^{-1}y^*$$

and that

$$Var(\hat{\tau}) = \sigma^2 C^{-1}$$
where
\[ C = X_2^\dagger [V^{-1} - V^{-1}X_1(X_1^\dagger V^{-1}X_1)^{-1}X_1^\dagger V^{-1}]X_2 \]  

(2.5)

The matrix \( C \) will be called the information matrix for \( \tau \).

We now need to find a balanced measurement design for which the average variance of the estimates of the values of the unknown specimens is minimized. This is equivalent to minimizing \( \text{Trace}(C^{-1}) \) within the class of balanced measurement designs for a fixed \( N \).

Kiefer (1975) provided a methodology which can be used to find optimal designs for various classes of problems. A key step in his approach depends on the convexity of the trace of the inverse of a positive definite matrix. The following result, which is a consequence of a well known convexity property of positive definite matrices (see Theorem 1.1.12, Fedorov (1972)), supplies the condition needed to apply Kiefer's method.

**Lemma 2.1:** For a given information matrix \( C \) described in (2.5), we have
\[ \text{Trace}(\tilde{C})^{-1} \leq \text{Trace}(C^{-1}) \]

where \( \tilde{C} = (\tilde{C})_{i,j} \) with
\[
\tilde{C}_{i,j} = \begin{cases} 
\frac{2}{m(m-1)} \sum_{k \neq l} C_{k,l} & \text{for } i \neq j \\
\frac{1}{m} \sum_{k=1}^{m} C_{k,k} & \text{for } i = j 
\end{cases} \]  

(2.6)

Clearly, \( \tilde{C} \) is of the form \( xI_m + yJ_m \) where \( I_m \) is an identity matrix, \( J_m \) is a \( m \times m \) matrix with all elements equal to 1. In fact, it is easy to see that the information matrix \( C \) corresponding to any balanced measurement design must have this form. Such matrices are often called completely symmetric because they are invariant under all permutations of the row-column labels. Therefore, to obtain an optimum balanced measurement design, it suffices to consider information matrices that are completely symmetric. By virtue of Lemma 2.1 it follows that a design that is optimum within the class of balanced designs is sometimes optimum within the class of all designs. This is the essence of the following corollary.

**Corollary 2.1:** Suppose that among all values of \( x \) and \( y \) for which \( xI_m + yJ_m \) is positive definite, \( \text{Trace}(xI_m + yJ_m)^{-1} \) is minimized by choosing \( x = x^* \) and \( y = y^* \). Further suppose that there exists a measurement design \( D^* \) whose information matrix is equal to \( x^*I_m + y^*J_m \). Then \( D^* \) is balanced and is A-optimum for estimating \( \tau \) in the class of all measurement designs.

A general expression for \( \text{Trace}(C^{-1}) \) will be useful in the quest for finding optimum balanced designs in our problem. We discuss this next.

**The structure of the information matrix for balanced designs**

We first introduce some notation and then describe the structure of the information matrix \( C \) for balanced measurement designs.

**Notation:**
- \( \epsilon_i \) = the number of times unknown \( i \) is the first observation plus the number of times unknown \( i \) is the last observation, i.e., \( \epsilon_i = \delta_{1,i} + \delta_{N,i} \). Note that \( \sum_{i=1}^{n} \epsilon_i = 0, 1, \) or 2.
\[ q_i = \text{the number of times two consecutive observations are of the unknown } i, \text{ i.e., } q_i = \sum_{k=1}^{N-1} \delta_{k,i} \delta_{k+1,i}. \]

\[ r_{i,j}^a = \text{the number of the times an observation of unknown } i \text{ follows directly after an observation of unknown } j, \text{ i.e., } r_{i,j}^a = \sum_{k=1}^{N-1} \delta_{k,j} \delta_{k+1,i}. \]

\[ r_{i,j}^b = \text{the number of the times an observation of unknown } j \text{ follows directly after an observation of unknown } i, \text{ i.e., } r_{i,j}^b = \sum_{k=1}^{N-1} \delta_{k,i} \delta_{k+1,j}. \]

\[ r_{i,j} = \text{the number of times unknowns } i \text{ and } j \text{ occur as neighboring pairs in the design.} \]

Thus \( r_{i,j} = r_{i,j}^a + r_{i,j}^b \).

The following example is given to illustrate these definitions.

**Example 2.2:** Consider the same sequence of observations as in Example 2.1,

\[ U_1 U_2 U_3 U_4 U_5 U_2 U_1 U_2 U_2 SS \]

- \( e_1 = 1 \) (the first observation is of the unknown specimen \( U_1 \))
- \( e_2 = 0 \) (neither the first nor the last observation is of \( U_2 \))
- \( e_3 = 0 \) (neither the first nor the last observation is of \( U_3 \))
- \( q_1 = 0 \) (no two consecutive observations are of \( U_1 \))
- \( q_2 = 1 \) (due to observations (10 & 11))
- \( q_3 = 2 \) (due to the pairs of observations (5 & 6) and (6 & 7))
- \( r_{1,2} = r_{1,2}^a + r_{1,2}^b = 1 + 1 = 2 \) (due to the pairs of observations (8 & 9) and (9 & 10))
- \( r_{1,3} = r_{1,3}^a + r_{1,3}^b = 0 + 2 = 2 \) (due to the pairs of observations (1 & 2) and (4 & 5))
- \( r_{2,3} = r_{2,3}^a + r_{2,3}^b = 1 + 0 = 1 \) (due to observations (7 & 8))

The parameters \( e_i, q_i, r_{i,j} \) describe the arrangement of observations on the unknowns and the standard and there are certain interrelationships among them which need to be recognized. These interrelationships are summarized in the following Lemma.

**Lemma 2.2:** Let

\[ t = \frac{1}{m} \sum_i^m t_i, \quad e = \frac{1}{m} \sum_i^m e_i, \quad q = \frac{1}{m} \sum_i^m q_i, \quad r = \frac{1}{(m)} \sum_{i<j}^m r_{i,j}. \]

For any measurement design the following relationships among the parameters must hold.

\[ \binom{m}{2} r + mq = mt - (b - b_0) \quad (2.7) \]

\[ \text{maximum} \{ 2 - me, b - mt \} \leq b_0 \leq b - 1 \quad (2.8) \]

\[ \text{maximum} \{ 0, \frac{m - (b - b_0)}{\binom{m}{2}} \} \leq r \leq \frac{mt - (b - b_0)}{\binom{m}{2}} \quad (2.9) \]

The proof is based on simple combinatorial arguments and is omitted.
The following Lemma describes the elements of the information matrix $C$ corresponding to an arbitrary measurement design.

**Lemma 2.3:** Let $D$ denote an arbitrary measurement design described by the parameters $e_i, q_i, t_i, b_0, b$ and $N$. Let $C$ denote the information matrix for $\tau$ under the design $D$. Then the elements of $C = (C_{ij})$, $i, j = 1, 2, \ldots, m$ are given by

$$
C_{ij} = \begin{cases}
    g_i - \frac{(1-\phi)s_i^2}{h} & \text{if } i = j \\
    -r_{ij}\phi - \frac{h(1-\phi)s_is_j}{h} & \text{if } i \neq j
\end{cases}
$$

(2.10)

where

$$
\begin{align*}
g_i &= t_i(1 + \phi^2) - 2q_i\phi - e_i\phi^2 \\
s_i &= t_i(1 - \phi) + e_i\phi \\
h &= 2 + (\sum_i t_i + b - 3)(1 - \phi)
\end{align*}
$$

The following Lemma describes conditions that must be satisfied by the design parameters $e_i, q_i, t_i$, and $r_{ij}$ in order for a measurement design to be balanced. It also gives the information matrix corresponding to balanced designs.

**Lemma 2.4:** A measurement design is balanced for all values of $\phi (-1 < \phi < 1)$ if and only if, for all $i$ and $j$, $t_i = t$, $q_i = q$, $e_i = e$, and $r_{ij} = r$. When this holds, the matrix $C$ is given by $C = xI_m + yJ_m$, where

$$
x = t(1 - \phi)^2 + \frac{2(b - b_0)}{m}\phi + m\phi - e\phi^2
$$

(2.11)

$$
y = -r\phi - \frac{(1 - \phi)(t(1 - \phi) + e\phi)^2}{2 + (mt + b - 3)(1 - \phi)}
$$

(2.12)

and the trace of $C^{-1}$ can be explicitly expressed as

$$
\text{Trace}(C^{-1}) = \frac{m - 1}{x} + \frac{1}{x + my}
$$

(2.13)

The proof involves straightforward algebra and is omitted.

According to the above lemma, $e_i$ must all be equal to a common value $e$ for a balanced design. Also, the sum of the $e_i$'s cannot be greater than 2. Therefore, when $m \geq 3$, each $e_i$ must be zero, i.e., $e$ must equal zero.

The following lemma gives a necessary and sufficient condition for the existence of a balanced measurement design corresponding to specified values of $m$, $b$, and $t$.

**Lemma 2.5:** Suppose $m \geq 3$. A balanced measurement design exists corresponding to specified values of $m$, $b$, and $t$, if and only if there exist nonnegative integers $q$ and $r$ with $0 \leq q \leq t - 1$ such that

$$
2 + mt - b \leq mq + m(q - 1)r/2 \leq mt - 1.
$$

The proof of this lemma follows from (2.7), (2.8), (2.9), the fact that $e = 0$ when $m \geq 3$, and the requirement for $q, r, b_0$ to be nonnegative integers satisfying the conditions $0 \leq q \leq t - 1$ and $2 \leq b_0 \leq b - 1$.  

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As stated earlier, we seek A-optimal designs within the class of balanced designs. This is equivalent to minimizing the quantity $\text{Trace}(C^{-1})$ in (2.13). Because of the balance, this amounts to minimizing the variance of the estimated value of each unknown within the class of balanced designs. By virtue of the above Lemmas, the problem has been reduced to minimizing the right-hand side of (2.13) with respect to $e, b_0$, and $r$, subject to the constraints given in (2.7), (2.8), and (2.9). In this paper we only present the results for the case where the number of unknown specimens is 3 or more. Results for the cases when the number of unknowns is at most 2 can be obtained using similar arguments. Interested reader can obtain the details from Taylor (1989).

3 A-optimum balanced designs for three or more unknowns

We begin this section with a lemma that gives an explicit expression for $\text{Trace}(C^{-1})$ for balanced designs with $m \geq 3$.

**Lemma 3.1:** Let $D$ be a balanced measurement design for three or more unknown specimens with $b_0$ empty batches and $r_{ij} = r$ for all $i, j$. Then the trace of the inverse of the information matrix $C$ is given by

$$\text{Trace}(C^{-1}) = \frac{m-1}{t(1-\phi)^2 + \frac{2(b-b_0)}{m} + mr\phi} + \frac{1}{t(1-\phi)^2 + \frac{2(b-b_0)}{m} + \frac{mt^2(1-\phi)\phi}{2+(mt+b-8)(1-\phi)}} \quad (3.1)$$

Note that, $N$, the total number of measurements, is equal to the number of measurements on the standard plus $m$ times the number of measurements on each unknown specimen. This yields the relation

$$mt + (b-1) = N = \text{Total number of observations}$$

So for fixed values of $m$, and $N$, the right hand side of (3.1) may be regarded as a function of $b_0$, $t$, and $r$. We minimize this function with respect to $b_0$ and $r$ for each allowable value of $t$, thus finding optimal balanced designs for each allowable combination of values of $b$ and $t$. The global optimum balanced design is then the best design among the set of optimum balanced designs obtained for the different admissible values of $b$ and $t$. We state the following two results, one for the case $-1 < \phi < 0$ and the other for the case $0 < \phi < 1$. Proofs are given in the appendix.

**Theorem 3.1:** Suppose $m$, the number of unknown specimens, is greater than or equal to 3 and $-1 < \phi < 0$, where $\phi$ is the parameter in the AR(1) model for the errors. Suppose each unknown specimen is to be measured $t$ times and that the total number of measurements, including those on the standard, is $N$. Assume the condition of Lemma 2.5 is satisfied so that the class of balanced measurement designs for the given $m$, $t$, and $b$ is nonempty. The values of $b_0$ and $r$ corresponding to an optimal balanced design are as follows.

1. If $b - 2 \geq m$ and $m$ is odd, then $b_0 = b - m$ and $r = 0$.

2. If $b - 2 \geq m$ and $m$ is an even number greater than $2t$, then $b_0 = b - m$ and $r = 0$.

3. If $b - 2 \geq m$ and $m$ is an even number less than or equal to $2t$, then the balanced optimum design is obtained from one of the following two possibilities:

   (i) $b_0 = b - m$ and $r = 0$, or (ii) $b_0 = b - m/2$ and $r = 1$. 

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The choice is to be made by numerically comparing the average variances corresponding to each of these cases and the result can depend on the value of $\phi$.

(4) If $m/2 \leq b - 2 < m$ and $m$ is an even integer less than or equal to $2t$, then $b_0 = b - m/2$ and $r = 1$.

(5) In all other cases balanced designs do not exist.

**Theorem 3.2:** Suppose $m$, the number of unknown specimens, is greater than or equal to 3 and $0 < \phi < 1$ where $\phi$ is the AR(1) parameter in the model for the errors. Suppose each unknown specimen is to be measured $t$ times and that the total number of measurements, including those on the standard, is $N$. Further assume that the condition of Lemma 2.5 is satisfied so that the class of balanced measurement designs is nonempty. The values of $b_0$ and $r$ corresponding to an optimal balanced design are as follows.

(1) If $m$ is even and $1/2 \leq (b - 2)/m \leq t$, then the optimum balanced design is obtained from one of the following four possibilities. The four possible designs given below must be numerically compared to pick the best among them. The result will generally depend on the value of $\phi$.

(a) Suppose the interval given by
\[
\text{maximum}\{0, \frac{2(m - b + 2)}{m(m - 1)}\} \leq r \leq \frac{2(mt - b + 2)}{m(m - 1)}
\]
contains at least one even nonnegative integer. Then a candidate for an optimum balanced design has $b_0 = b - mx_0$ and $r = r_0$ where $r_0$ is the largest even integer in the interval in (3.2) and $x_0$ is the largest positive integer less than or equal to $(b - 2)/m$. Note that this case can occur only when $(b - 2)/m \geq 1$.

(b) Suppose the interval in (3.2) contains at least one nonnegative odd integer. Then a candidate for an optimum balanced design has $b_0 = b - mx_0$ and $r = r_0$ where $r_0$ is the largest odd integer in the interval given by (3.2), and $x_0$ is the largest positive odd multiple of $1/2$ less than or equal to $(b - 2)/m$.

(c) Suppose the interval given by
\[
\frac{2(mt - b + 2)}{m(m - 1)} < r \leq \frac{2(mt - 1)}{m(m - 1)}
\]
contains at least one nonnegative even integer. Then a candidate for an optimum balanced design has $b_0 = b - mx_0$ and $r = r_0$ where $r_0$ is the smallest even integer in the interval given by (3.3) and
\[
x_0 = t - \frac{(m - 1)r_0}{2}
\]

(d) Suppose the interval in (3.3) contains at least one odd integer. Then a candidate optimum balanced design has $b_0 = b - mx_0$ and $r = r_0$ where $r_0$ is the smallest odd integer in the interval in (3.3) and
\[
x_0 = t - \frac{(m - 1)r_0}{2}
\]

(2) If $m$ is odd and $1 \leq (b - 2)/m \leq t$, then the optimum design is given by one of the following two possibilities. They must be numerically compared and the better one must be chosen. The result will generally depend on the value of $\phi$.
(a) Suppose the interval in (3.2) contains at least one nonnegative integer. Then a candidate optimum balanced design has \( b_0 \) and \( r_0 \) where \( r_0 \) is the largest integer in the interval given by (3.2), and \( x_0 \) is the largest integer less than or equal to \((b - 2)/m\).

(b) Suppose the interval in (3.3) contains at least one nonnegative integer. Then a candidate optimum balanced design has \( b_0 \) and \( r_0 \) where \( r_0 \) is the smallest integer in the interval given by (3.3) and \( x_0 = t - \frac{(m-1)r_0}{2} \).

(3) If \((b - 2)/m > t\), then the optimum balanced design has \( b_0 = b - mt \) and \( r = 0 \).

(4) In all remaining cases a balanced design does not exist.

4 An algorithm to construct balanced measurement designs

For given values of \( m, N \), and \( t \), we gave in the previous section the values of \( r \) and \( b_0 \) which minimize \( \text{Trace}(C^{-1}) \). It remains to show how to construct the desired balanced designs corresponding to \( m, t, r \) and \( b_0 \). For our construction, we will need to use a special class of latin squares which were considered by Kiefer and Wynn (1981) in their study of equineighbored designs. Also see Cheng (1983).

For a given integer \( m \), consider the \( m \times m \) array \( A \) whose \((j, l)\) element \((1 \leq j, l \leq m)\) is the symbol \( U_p \) where

\[
p - 1 = \left[ \sum_{i=1}^{j} (-1)^i (i - 1) + \sum_{i=1}^{l} (-1)^i (i - 1) \right] \mod m
\]

\[(4.1)\]

It is easily verified that \( A \) has the following properties.

(1) \( A \) is a latin square. Each column or each row of \( A \) contains all \( m \) different symbols (which represent the \( m \) unknown specimens) exactly once.

(2) When \( m \) is an odd number, \( A \) is symmetric. When \( m \) is an even number, then \( A \) is symmetric with respect to the two leading diagonals, i.e., \( a_{j,l} = a_{l,j} = a_{m+1-j,m+1-l} = a_{m+1-l,m+1-j} \).

(3) For \( m \) odd, each pair of symbols appear as neighbors exactly once in the rows of the first \( m \times \frac{m + 1}{2} \) subarray.

(4) For \( m \) even, each pair of symbols appear as neighbors exactly once in the rows of the first \( \frac{m}{2} \times m \) subarray and also in the first \( m \times \frac{m}{2} \) subarray.

The following arrays are given to illustrate these results.
Example 4.1: For \( m = 5 \) and 6, the arrays obtained from (4.1) are, respectively,

\[
\begin{array}{cccccc}
U_5 & U_1 & U_4 & U_2 & U_3 \\
U_1 & U_2 & U_5 & U_3 & U_4 \\
U_4 & U_5 & U_3 & U_1 & U_2 \\
U_2 & U_3 & U_1 & U_4 & U_5 \\
U_3 & U_4 & U_2 & U_6 & U_1 \\
U_5 & U_4 & U_2 & U_6 & U_1 \\
\end{array}
\quad \quad \begin{array}{cccccc}
U_6 & U_1 & U_5 & U_2 & U_4 & U_3 \\
U_2 & U_6 & U_3 & U_5 & U_4 & U_1 \\
U_5 & U_6 & U_4 & U_1 & U_3 & U_2 \\
U_3 & U_5 & U_1 & U_4 & U_6 & U_2 \\
U_4 & U_5 & U_3 & U_6 & U_2 & U_1 \\
U_5 & U_4 & U_3 & U_6 & U_1 & U_2 \\
\end{array}
\]

Based on the arrays produced by (4.1), we present the following algorithm to construct balanced measurement designs. We consider three separate cases: (A) \( r = 0 \), (B) \( r > 0 \) with \((m-1)r\) odd, and (C) \( r > 0 \) with \((m-1)r\) even.

The Algorithm:

Case (A): Suppose \( r = 0 \). Then \( mq = mt - (b - b_0) \) and \( k = (b - b_0)/m \) must be an integer. In particular \( q = t - k \). Let \( t = uk + v \) where \( u \) and \( v \) are integers and \( 0 \leq v < k \). Construct an array \( D \) (not necessarily a rectangular array), with \( mk \) rows such that, for each \( i \) with \( 1 \leq i \leq m \), there are \( k - v \) rows consisting only of \( u \) occurrences of \( U_i \) and \( v \) rows consisting only of \( u + 1 \) occurrences of \( U_i \). To this array, add an initial column consisting of \( mk \) standards, and also add a single standard after the last element of the last row. Concatenate all the rows of this array to produce a single row consisting of \( m(k - v)u + mv(u + 1) + mk + 1 = N \) symbols. If \( b_0 = 2 \), then this is the required measurement design. If \( b_0 > 2 \) then add \( b_0 - 2 \) additional standards to the current design sequence by placing each additional standard next to an already occurring standard. This can usually be done in many different ways and each one will lead to a design satisfying the requirements.

Case (B): Suppose \( r > 0 \) and \((m-1)r\) is an even integer. Thus either \( m \) is odd or \( m \) and \( r \) are both even. We must have \( b - b_0 = km \) for some integer \( k \). The following steps lead to a balanced measurement design meeting the requirements and with (nearly) equal batch sizes for the nonempty batches.

Step (1): For a given \( m \), let \( A \) be the \( m \times m \) array obtained from (4.1). If \( m \) is odd, then let \( m_1 = (m+1)/2 \), otherwise \( m_1 = m/2 \). Let \( A_1 \) be the first \( m \times m_1 \) subarray of \( A \) and \( A_2 \) be the \( m \times m_1 \) array which is the “reflection” of \( A_1 \), i.e., \( A_2 \) is obtained by permuting the columns of \( A_1 \) according to the permutation

\[
\begin{pmatrix}
1 & 2 & 3 & \cdots & m_1 - 1 & m_1 \\
m_1 & m_1 - 1 & m_1 - 2 & \cdots & 2 & 1
\end{pmatrix}
\]

Now we define an operation for merging two arrays by columns. Let \( B = B_1 : b \) and \( C = c : C_1 \) be two arrays of sizes \( m_0 \times l_1 \) and \( m_0 \times l_2 \), respectively, and \( b \) and \( c \) are column vectors. Then the operation \( \circ \) is defined by

\[
B \circ C = \begin{cases}
B_1 : b ; c & \text{if } b = c \\
B_1 : b ; c : C_1 & \text{if } b \neq c
\end{cases}
\]

Let the array \( D_1 = A_1 \). If \( r > 1 \), then for \( j \geq 2 \) recursively define \( D_j = D_{j-1} \circ A_1 \) if \( j \) is odd and \( D_j = D_{j-1} \circ A_2 \) if \( j \) is even. By using properties (3) and (4) of \( A \) described previously and mathematical induction, it is easy to verify that each pair of unknown specimens appears as neighbors exactly \( r \) times in the \( m \) rows of the array \( D_r \). Furthermore, no unknown occurs next to itself in any of the \( m \) rows. Note also that \( D_r \) is an array of size \( m \times n_1 \), where \( n_1 = 1 + (m-1)r/2 \).
Step (2): If \( q \) is equal to 0 then go to Step (3). Suppose \( q \) is greater than 0. Let \( c_1, \ldots, c_n \) be the \( n_1 \) columns of \( D_r \). Enlarge the current array \( D_r \) by repeating selected columns of \( D_r \) next to themselves such that the number of columns in the enlarged array is \( q + n_1 = q + 1 + (m - 1)r/2 \). It makes no difference as to which columns are selected to be repeated or how many times a given column is repeated as long as the total number of new columns added is \( q \). At the end of this step each unknown specimen occurs in the array exactly \( n = q + 1 + (m - 1)r/2 \) times. This follows from the fact that each column of \( D_r \) contains each unknown exactly once.

Step (3): If \( k = 1 \) then go to Step (4). Suppose \( k > 1 \). Let \( k_0 = k - 1 \). Consider integers
\[
1 \leq i_1 < i_2 < \cdots < i_{k_0-1} < i_{k_0} \leq n
\]
For each \( j = 1, \ldots, k_0 \), replace column \( c_{ij} \) in \( D_r \) by the block of three columns \( I_{large} c_{ij} | s | c_{ij} \) where \( s \) is a column of \( S \)'s representing measurements of a standard. The resulting modified array \( D_r \) will now have \( n + k - 1 = t \) columns consisting of unknown specimens and \( k - 1 \) columns consisting of standards only.

Step (4): Add a column \( s \) of standards as the first row of \( D_r \) and also add a single standard to the right of the last element of the last row. The total number of standards in this modified (non-rectangular) array is \( mk + 1 = (b - 1) - (b_0 - 2) \). Concatenate the rows of this array to produce a single row consisting of standards and unknowns. If \( b_0 = 2 \), then this row, when viewed as a measurement design, meets all the requirements. If \( b_0 > 2 \) then the number of standards occurring in the current array \( D_r \) is less than the required number by an amount equal to \( b_0 - 2 \) as is the number of empty batches. This can be rectified by including \( b_0 - 2 \) additional standards such that each of the added standard is placed adjacent to an already occurring standard. This also creates \( b_0 - 2 \) additional empty batches. This final row consisting of unknowns and standards is then a balanced measurement design meeting all the requirements.

Note: The batch sizes in this design depend on how the columns \( i_1 < \cdots < i_{k_0} \) are chosen. Let \( t = (k - 1)u + v \) where \( u \) and \( v \) are nonnegative integers and \( |u - v| \) is as small as possible. For \( j = 1, \ldots, k_0 \), choose \( i_j = ju - j + 1 \). Then the resulting measurement design will have \( (k - 1)m \) batches of size \( u \) and \( m \) batches of size \( v \) and thus will have nearly equal batch sizes. Other choices of \( i_1, \ldots, i_{k_0} \) are also possible.

Case (C): Now suppose \( r > 0 \) and \( (m - 1)r \) is odd. In this case \( b - b_0 = km/2 \), where \( k \) is an odd positive integer. The following steps will lead to a (nearly) equal batch-size design.

Step (1): Let \( A \) be the \( m \times m \) array obtained from (4.1). Let \( A_1 \) be the \( m/2 \times m \) array of \( A \) consisting of the first \( m/2 \times m \) subarray of \( A \). Also let \( A_2 \) be the \( m/2 \times m \) array that is the “reflection” of \( A_1 \) as described earlier.

Let the array \( D_1 = A_1 \). If \( r > 1 \), then for \( j \geq 2 \) define \( D_j \) recursively by \( D_j = D_{j-1} \circ A_1 \) if \( j \) is odd, and \( D_j = D_{j-1} \circ A_2 \) if \( j \) is even. Each pair of unknown specimens appears as neighbors exactly \( r \) times in the \( m/2 \) rows of the array \( D_r \). Also \( D_r \) is an array of size \( m/2 \times n_1 \), where \( n_1 = m + (m - 1)(r - 1) \).

Step (2): If \( q \) equals zero, then go to Step (3). Suppose \( q > 0 \). By using properties (1) and (2) of the array \( A \) described previously, it is easily checked that for each \( i, i = 1, \ldots, n_1/2 \), the pair of columns, column \( i \) and column \( n_1 + 1 - i \), together contains all \( m \) different unknown specimens exactly once. Now enlarge the current array \( D_r \) by repeating next to themselves selected pairs of columns, column \( i \) and column \( n_1 + 1 - i \) for various \( i \), such that the total number of additional pairs of columns added is \( q \). It makes no difference which pairs of columns are selected to be repeated or how many times a given pair of columns is repeated so long as the total number of added pairs is \( q \).
At this point the array $D_r$ has $m/2$ rows and $n = n_1 + 2q$ columns. We also note that, for each $i$, the unknown $U_i$ occurs next to itself exactly $q$ times among its rows. Moreover, each unknown occurs in the array exactly $q + n_1/2 = q + m/2 + (m-1)(r-1)/2$ times. Since $t = q + n_1/2 + (k-1)/2$ we need $(k-1)/2$ additional observations on each unknown.

Step (3): If $k = 1$ then go to Step (4). Suppose $k > 1$. The current array $D_r$ is of size $m/2 \times n$, where $n = 2q + m + (m-1)(r-1)$. Each pair of columns, $i$ and $n + 1 - i$, still contains all $m$ different unknown specimens, for $i = 1, 2, \ldots, n/2$. Let $k_0 = (k-1)/2$. Suppose

$$1 \leq i_1 < i_2 < \cdots < i_{k_0-1} < i_{k_0} \leq n/2.$$ 

For each $j = i_1, \ldots, i_{k_0}$, replace columns $c_j$ and $c_{n+1-j}$ by a block of 3 columns, $c_j | s | c_i$ and $c_{n+1-j} | s | c_{n+1-j}$, respectively. At the end of this step each unknown specimen occurs exactly $t$ times in the rows of the modified array $D_r$.

Step (4): Add a column of $S$'s before the first column of the current array $D_r$ and a single $S$ following the element in the last row and last column. This yields a (nonrectangular) array with $m$ rows. Concatenate the rows of this array to produce a single row of standards and unknowns. This leads to a balanced measurement design meeting all requirements except that it has $b_0 - 2$ fewer measurements on standards than what is required and also has $b_0 - 2$ fewer empty batches. If $b_0 = 2$ then we are done. If $b_0 > 2$, then we introduce $b_0 - 2$ additional standards in the design sequence by placing them adjacent to already occurring standards. Many different choices will be available here but any one of them will work. This yields the final design.

Note: The choice of the columns $i_1 < i_2 < \cdots < i_{k_0}$ in Step (3) determines the batch sizes in the final design. Let $2t = (k-1)u + v$ where $u$ and $v$ are nonnegative integers and $|u - v|$ is as small as possible. Choose $i_j = j u - (j-1) v$ for $j = 1, \ldots, k_0$. This choice leads to $(k-1)m/2$ batches of size $u$ and $m/2$ batches of size $v$, thus producing nearly equal batch sizes. Other choices of the columns are also possible leading to a different definition of batches.

The following three examples are given to illustrate the algorithm.

**Example 4.2:** Suppose $m = 5$, $r = 0$, $q = 3$, $t = 5$, $b = 12$, and $b_0 = 2$. A balanced measurement design with these parameters can be constructed according to Case (A) of the algorithm above. Note that the value of $k$ here is 2 and also that $t = 5 = u k + v$ with $u = 2$ and $v = 1$. Hence construct the following array $D$ first.

$$
D = \begin{pmatrix}
U_1 & U_1 & U_1 \\
U_2 & U_3 & U_2 \\
U_3 & U_3 & U_3 \\
U_4 & U_4 & U_3 \\
U_5 & U_5 & U_3
\end{pmatrix}
$$
After adding the standards we get

\[ D = \]

\[ S \ U_1 \ U_1 \\
S \ U_1 \ U_1 \ U_1 \\
S \ U_2 \ U_2 \\
S \ U_3 \ U_2 \ U_2 \\
S \ U_3 \ U_3 \\
S \ U_4 \ U_3 \ U_3 \\
S \ U_4 \ U_4 \ U_3 \\
S \ U_4 \ U_4 \ U_4 \\
S \ U_4 \ U_5 \\
S \ U_4 \ U_5 \ U_5 \ U_5 \ S \]

Concatenating the rows of the above array gives us the required measurement design, viz.,

\[ S \ U_1 \ U_1 \ S \ U_1 \ U_1 \ U_1 \ S \ U_2 \ U_2 \ S \ U_2 \ U_2 \ U_2 \ S \ U_2 \ U_2 \ U_2 \ S \ U_3 \ U_3 \ S \ U_3 \ U_3 \ U_3 \ \]

\[ U_4 \ U_4 \ S \ U_4 \ U_4 \ U_4 \ S \ U_4 \ U_4 \ U_4 \ U_4 \ S \ U_5 \ U_5 \ S \ U_5 \ U_5 \ U_5 \ U_5 \ U_5 \ S \]

**Example 4.3**: Suppose \( m = 5 \), \( r = 3 \), \( q = 1 \), \( t = 9 \), \( b = 14 \) and \( b_0 = 4 \). A balanced measurement design satisfying these parameters can be obtained from Case (B) of the algorithm described above.

**Step (1)**: From Example 4.1,

\[ A_1 A_2 = \]

\[ U_5 \ U_1 \ U_4 : U_4 \ U_1 \ U_5 \\
U_1 \ U_2 \ U_5 : U_5 \ U_2 \ U_1 \\
U_2 \ U_3 \ U_3 : U_3 \ U_5 \ U_4 \\
U_3 \ U_4 \ U_2 : U_2 \ U_4 \ U_3 \]

Since \( r = 3 \),

\[ D_r = A_1 A_2 A_1 = \]

\[ U_5 \ U_1 \ U_4 \ U_1 \ U_5 \ U_1 \ U_4 \ U_4 \\
U_1 \ U_2 \ U_5 \ U_2 \ U_1 \ U_2 \ U_5 \ U_5 \\
U_2 \ U_3 \ U_3 \ U_1 \ U_3 \ U_2 \ U_5 \ U_4 \\
U_3 \ U_4 \ U_2 \ U_4 \ U_3 \ U_4 \ U_4 \ U_2 \]

**Step (2)**: Since \( q = 1 \), repeating the last column of the current \( D_r \) gives

\[ D_r = \]

\[ U_5 \ U_1 \ U_4 \ U_1 \ U_5 \ U_1 \ U_4 \ U_4 \\
U_1 \ U_2 \ U_5 \ U_2 \ U_1 \ U_2 \ U_5 \ U_5 \\
U_2 \ U_3 \ U_3 \ U_1 \ U_3 \ U_2 \ U_5 \ U_4 \\
U_3 \ U_4 \ U_2 \ U_4 \ U_3 \ U_4 \ U_4 \ U_2 \]

**Step (3)**: \( b - b_0 = 10 = km \), with \( k = 2 \). Since \( t = 9 \), we have \( u = 5 \) and \( v = 4 \). The 5th column

\[ U_5 \\
U_1 \\
U_4 \\
U_2 \\
U_3 \]

"15"
is replaced by the block of three columns

\[
\begin{array}{ccccccc}
U_6 & S & U_5 \\
U_5 & S & U_4 \\
U_4 & S & U_3 \\
U_3 & S & U_2 \\
U_2 & S & U_1 \\
U_1 & S & U_0 \\
\end{array}
\]

and we obtain the array

\[
\begin{array}{ccccccccccccccc}
U_6 & U_1 & U_4 & U_3 & U_2 & S & U_5 & U_1 & U_4 & U_4 \\
U_5 & U_2 & U_5 & U_3 & U_4 & S & U_1 & U_2 & U_5 & U_5 \\
U_4 & U_3 & U_6 & U_5 & U_4 & S & U_3 & U_4 & U_5 & U_3 \\
U_3 & U_4 & U_7 & U_6 & U_5 & U_4 & S & U_2 & U_3 & U_1 \\
U_2 & U_5 & U_8 & U_7 & U_6 & U_5 & S & U_3 & U_4 & U_2 \\
U_1 & U_6 & U_9 & U_8 & U_7 & U_6 & S & U_3 & U_4 & U_2 \\
\end{array}
\]

Step (4): Add a column of $S$'s before the first column and a single $S$ at the end of the last row and get the following nonrectangular array:

\[
\begin{array}{ccccccccccccccc}
S & U_6 & U_1 & U_4 & U_3 & U_2 & S & U_5 & U_1 & U_4 & U_4 \\
S & U_1 & U_2 & U_5 & U_4 & U_3 & S & U_1 & U_2 & U_5 & U_5 \\
S & U_4 & U_3 & U_6 & U_5 & U_4 & S & U_3 & U_4 & U_3 & U_3 \\
S & U_2 & U_5 & U_8 & U_7 & U_6 & U_4 & S & U_2 & U_3 & U_1 \\
S & U_3 & U_6 & U_9 & U_8 & U_7 & U_6 & S & U_3 & U_4 & U_2 \\
\end{array}
\]

Concatenating the rows of this array produces the following design.

\[
\begin{array}{ccccccccccccccc}
S & U_6 & U_1 & U_4 & U_3 & U_2 & S & U_5 & U_1 & U_4 & U_4 & S & U_5 & U_1 & U_4 & U_4 \\
S & U_1 & U_2 & U_5 & U_4 & U_3 & S & U_1 & U_2 & U_5 & U_5 & S & U_1 & U_2 & U_5 & U_5 \\
S & U_4 & U_3 & U_6 & U_5 & U_4 & S & U_3 & U_4 & U_3 & U_3 & S & U_3 & U_4 & U_3 & U_3 \\
S & U_2 & U_5 & U_8 & U_7 & U_6 & U_4 & S & U_2 & U_3 & U_1 & S & U_2 & U_3 & U_1 & U_1 \\
S & U_3 & U_6 & U_9 & U_8 & U_7 & U_6 & S & U_3 & U_4 & U_2 & S & U_3 & U_4 & U_2 & U_2 \\
\end{array}
\]

Since $b_0 = 4$, $b_0 - 2 = 2$, and we add two additional standards each adjacent to a previously occurring standard. The final design is given below.

\[
\begin{array}{ccccccccccccccc}
S & U_6 & U_1 & U_4 & U_3 & U_2 & S & U_5 & U_1 & U_4 & U_4 & S & U_5 & U_1 & U_4 & U_4 \\
S & U_1 & U_2 & U_5 & U_4 & U_3 & S & U_1 & U_2 & U_5 & U_5 & S & U_1 & U_2 & U_5 & U_5 \\
S & U_4 & U_3 & U_6 & U_5 & U_4 & S & U_3 & U_4 & U_3 & U_3 & S & U_3 & U_4 & U_3 & U_3 \\
S & U_2 & U_5 & U_8 & U_7 & U_6 & U_4 & S & U_2 & U_3 & U_1 & S & U_2 & U_3 & U_1 & U_1 \\
S & U_3 & U_6 & U_9 & U_8 & U_7 & U_6 & S & U_3 & U_4 & U_2 & S & U_3 & U_4 & U_2 & U_2 \\
\end{array}
\]

**Example 4.4:** Suppose $m = 6$, $r = 3$, $g = 0$, $t = 10$, $b = 17$ and $b_0 = 2$. A balanced measurement design satisfying these parameters can be obtained from Case (C) of the algorithm as follows.

Step (1): From Example 4.1,

\[
A_1 : A_2 = \begin{array}{cccccccccc}
U_6 & U_1 & U_5 & U_2 & U_4 & U_3 & U_4 & U_2 & U_5 & U_1 & U_6 \\
U_1 & U_2 & U_6 & U_3 & U_4 & U_4 & U_4 & U_3 & U_6 & U_2 & U_1 \\
U_6 & U_5 & U_4 & U_1 & U_3 & U_2 & U_3 & U_1 & U_4 & U_6 & U_5 \\
\end{array}
\]

Since $r = 3$,

\[
D_r = A_1 \circ A_2 \circ A_1 = \begin{array}{ccccccccc}
U_6 & U_1 & U_5 & U_2 & U_4 & U_3 & U_4 & U_2 & U_5 & U_1 & U_6 \\
U_1 & U_2 & U_6 & U_3 & U_4 & U_4 & U_3 & U_6 & U_2 & U_1 \\
U_6 & U_5 & U_4 & U_1 & U_3 & U_2 & U_3 & U_1 & U_4 & U_6 & U_5 \\
\end{array}
\]

Step (2): $q = 0$. Keep the current array. We have $n_1 = 16$. 

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Step (3): \( b - b_0 = 15 = km/2 \), with \( k = 5 \). Since \( t = 10 \), we get \( 2t = (k - 1)4 + 4 \) so \( u = 4 \) and \( v = 4 \). Each row of \( D_r \) is split at the 4\(^{th}\), 7\(^{th}\), 10\(^{th}\) and 13\(^{th}\) elements and this gives

\[
\begin{align*}
U_6 & \quad U_1 & \quad U_3 & \quad U_2 & \quad U_4 & \quad S & \quad U_3 & \quad U_4 & \quad U_2 & \quad U_5 & \quad U_1 & \quad S & \quad U_1 & \quad U_4 & \quad U_1 & \quad U_5 & \quad S & \quad U_5 & \quad U_2 & \quad U_4 & \quad U_3 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_5 & \quad U_1 & \quad U_2 & \quad U_6 & \quad S & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \\
U_5 & \quad U_6 & \quad U_4 & \quad U_1 & \quad S & \quad U_1 & \quad U_3 & \quad U_2 & \quad U_3 & \quad S & \quad U_3 & \quad U_1 & \quad U_4 & \quad U_6 & \quad S & \quad U_6 & \quad U_5 & \quad U_6 & \quad U_4 & \quad S & \quad U_4 & \quad U_1 & \quad U_3 & \quad U_2 & \quad S
\end{align*}
\]

Step (4): Add a column of \( S \)'s before the first column and a single \( S \) at the end of the last row to get the following nonrectangular array.

\[
\begin{align*}
S & \quad U_6 & \quad U_1 & \quad U_3 & \quad U_2 & \quad S & \quad U_2 & \quad U_4 & \quad U_3 & \quad U_4 & \quad U_2 & \quad U_5 & \quad U_1 & \quad S & \quad U_1 & \quad U_6 & \quad U_1 & \quad U_5 & \quad S & \quad U_5 & \quad U_2 & \quad U_3 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_5 & \quad U_1 & \quad U_2 & \quad U_6 & \quad S & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \\
S & \quad U_6 & \quad U_4 & \quad U_1 & \quad S & \quad U_1 & \quad U_3 & \quad U_2 & \quad U_3 & \quad S & \quad U_3 & \quad U_1 & \quad U_4 & \quad U_6 & \quad S & \quad U_6 & \quad U_5 & \quad U_6 & \quad U_4 & \quad S & \quad U_4 & \quad U_1 & \quad U_3 & \quad U_2 & \quad S
\end{align*}
\]

Concatenating the rows of the above array we get the design sequence shown below.

\[
S \quad U_6 & \quad U_1 & \quad U_3 & \quad U_2 & \quad S & \quad U_2 & \quad U_4 & \quad U_3 & \quad U_4 & \quad U_2 & \quad U_5 & \quad U_1 & \quad S & \quad U_1 & \quad U_6 & \quad U_1 & \quad U_5 & \quad S & \quad U_5 & \quad U_2 & \quad U_3 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_5 & \quad U_1 & \quad U_2 & \quad U_6 & \quad S & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \quad U_5 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \quad U_5 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \quad U_5 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S & \quad U_3 & \quad U_6 & \quad U_3 & \quad U_5 & \quad U_4 & \quad U_5 & \quad U_3 & \quad U_4 & \quad U_2 & \quad S
\end{align*}
\]

Since \( b_0 = 2 \), no more standards need to be added.

**Example 4.4:**

## 5 Optimal balanced designs for a given cost

In this section, we discuss an example which shows how to use the results of sections 3 and 4 to help an investigator find optimal designs for a given cost.

**Example 5.1:** An investigator has made repeated observations on a standard and as a result she is confident that the measurement process follows the model described in (2.1) with unknown \( \mu \) and a first order autoregressive error structure. She is planning an experiment in which at least one observation is to be made on each of \( m \) different unknown specimens. Suppose \( \phi = 0.5 \), \( m = 6 \). Each measurement of a standard costs 3 dollars and of an unknown specimen costs 2 dollars, but the budget allows at most 60 dollars for the experiment. The investigator would like to determine the optimal combination of cost and precision for the experiment. For every affordable combination of \( t \) observations on the \( m \) unknowns and \( b - 1 \) observations
of a standard, we apply the results presented in section 3 to generate the following table.

<table>
<thead>
<tr>
<th>b</th>
<th>m</th>
<th>t</th>
<th>b₀</th>
<th>r</th>
<th>q</th>
<th>Var(\bar{v})/\sigma²</th>
<th>cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>6</td>
<td>4</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0.42328</td>
<td>60</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0.41313</td>
<td>60</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>3</td>
<td>5</td>
<td>1</td>
<td>0</td>
<td>0.41830</td>
<td>57</td>
</tr>
<tr>
<td>7</td>
<td>6</td>
<td>3</td>
<td>4</td>
<td>1</td>
<td>0</td>
<td>0.42415</td>
<td>54</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0.43082</td>
<td>51</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>3</td>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0.43850</td>
<td>48</td>
</tr>
<tr>
<td>13</td>
<td>6</td>
<td>2</td>
<td>7</td>
<td>0</td>
<td>1</td>
<td>0.88687</td>
<td>60</td>
</tr>
<tr>
<td>12</td>
<td>6</td>
<td>2</td>
<td>6</td>
<td>0</td>
<td>1</td>
<td>0.88783</td>
<td>57</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>2</td>
<td>5</td>
<td>0</td>
<td>1</td>
<td>0.88889</td>
<td>54</td>
</tr>
<tr>
<td>10</td>
<td>6</td>
<td>2</td>
<td>4</td>
<td>0</td>
<td>1</td>
<td>0.89006</td>
<td>51</td>
</tr>
<tr>
<td>9</td>
<td>6</td>
<td>2</td>
<td>3</td>
<td>0</td>
<td>1</td>
<td>0.89136</td>
<td>48</td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>2</td>
<td>2</td>
<td>0</td>
<td>1</td>
<td>0.89286</td>
<td>45</td>
</tr>
<tr>
<td>17</td>
<td>6</td>
<td>1</td>
<td>11</td>
<td>0</td>
<td>0</td>
<td>0.80702</td>
<td>60</td>
</tr>
</tbody>
</table>

In this table we have not listed all the possible designs with \( t = 1 \) because their performance is worse than the design with \( b = 17, t = 1 \). From the table, the investigator can determine the best compromise between precision and cost. Suppose she decides that an optimal design with a cost of 48 dollars gives her the best compromise between cost and precision. Thus, a design with the parameters \( b = 5, m = 6, t = 3, b₀ = 2, r = 1, \) and \( q = 0 \) is the required design. This design can be easily constructed by the algorithm provided in section 4 and it is given by

\[
SU_5U_1U_6U_2U_4SU_1U_2U_6U_5U_4SU_5U_6U_4U_1U_3U_2S
\]

6 Concluding remarks

In this paper we have carried out a detailed analysis of exact optimum balanced measurement designs assuming an AR(1) error structure. It is assumed that the number of unknowns is three or greater. When the number of unknowns is less than three the reader is referred to Taylor (1989). In principle the approach can be extended to higher order autoregressive error structures but an analytical treatment of exact optimum designs seems unfeasible. In these cases it may be necessary to consider approximately optimum designs. In practical applications low order AR(1) error models are often useful as approximations to the actual serial correlation structure. Thus the designs presented in this paper can provide useful information in these cases as well.

References


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Appendix

Proof of Theorem 3.1:

Suppose \(-1 < \phi < 0\). The equality in (2.7) implies that \(b - b_0 = mx\) for some \(x\) where \(x\) must be a positive integer when \((m-1)r\) is even and a positive odd multiple of \(1/2\) when \((m-1)r\) is odd. We substitute \(b - b_0 = mx\) in the expression for the trace in (3.1) and

\[
\text{Trace}(C^{-1}) = \frac{m-1}{t(1-\phi)^2 + \frac{2\phi}{m} + m\phi} + \frac{1}{t(1-\phi)^2 + \frac{2\phi}{m} - \frac{m^2(1-\phi)^2}{2(mt+b-3)(1-\phi)}} \tag{A.1}
\]

We minimize this expression with respect to allowable values of \(x_0\) and \(r\) for each fixed \(t\). We consider several cases.

1. Suppose \(m\) is odd and \(b - 2 \geq m\). For a fixed \(r\), (A.1) is minimized by a small \(x\). Due to the constraints given in (2.7)-(2.9) and since \((m-1)r\) is even in this case for every allowable \(r\), \(x\) must be a positive integer in the interval

\[
\max \left\{ \frac{1}{m}, 1 - \frac{(m-1)r}{2} \right\} \leq x \leq \min \left\{ t - \frac{(m-1)r}{2}, \frac{b - 2}{m} \right\}.
\]

Hence \(x\) must be chosen to be 1. We substitute \(x = 1\) in the expression for the trace in (A.1) and minimize the resulting expression with respect to \(r\). Again, since \(\phi\) is negative, we must choose the smallest allowable value for \(r\). Since \(r\) must belong to the interval given by

\[
\max \left\{ 0, \frac{2(m-1)}{m(m-1)} \right\} \leq r \leq \frac{2(mt)}{m(m-1)}
\]

and since the lower bound for \(r\) in this case is zero, we take \(r = 0\). Therefore, we have \(r = 0\) and \(b_0 = b - m\).

2. Suppose \(m\) is an even number greater than \(2t\) and \(b - 2 \geq m\). Here we consider two subcases - \(r\) odd and \(r\) even.

If \(r\) is odd, then \((m-1)r\) is odd, so \(x\) must be an odd positive multiple of \(1/2\). However, since \(m\) is greater than \(2t\), it can be easily verified that there are no such values for \(x\) and hence a balanced design does not exist in this case.

If \(r\) is even, then \((m-1)r\) is even, so \(x\) must be a positive integer. As in case (1) \(x\) must be chosen to be 1. Substituting \(x = 1\) in (A.1) and minimizing with respect to \(r\) yields \(r = 0\). So the solution in this case is given by \(r = 0\) and \(b_0 = b - m\).

3. Suppose \(m\) is an even number less than or equal to \(2t\) and \(b - 2 \geq m\). Again we consider two subcases - \(r\) odd and \(r\) even.
If \( r \) is odd, then \((m - 1)r\) is odd, so \( x \) must be an odd positive multiple of 1/2. The smallest allowable value for \( x \) in this case is \( x = 1/2 \). Substituting \( x = 1/2 \) in (A.1) and minimizing with respect to \( r \) gives \( r = 1 \). Therefore the solution in this subcase is \( r = 1 \) and \( b_0 = b - m/2 \).

If \( r \) is even, then \((m - 1)r\) is even, so \( x \) must be a positive integer. As in case (2) \( x \) must be chosen to be 1. Substituting \( x = 1 \) in (A.1) and minimizing with respect to \( r \) yields \( r = 0 \). So the solution in this subcase is given by \( r = 0 \) and \( b_0 = b - m \).

Putting the two subcases together we find that the optimum design is the better of the two designs obtained in the two subcases.

(4) Here we have \( 1/2 \leq (b - 2)/m < 1 \) and \( m \) is an even integer less than or equal to \( 2t \). If \( r \) is an even integer we find that the set of allowable values for \( x \) is empty. So \( r \) must be chosen to be odd. For a fixed odd positive \( r \) the trace is minimized by taking \( x = 1/2 \). Substituting this in (A.1) and minimizing with respect to \( r \) gives \( r = 1 \). The solution in this case is then \( r = 1 \) and \( b_0 = b - m/2 \).

(5) Clearly no balanced design exists in the remaining cases because the set of allowable values for \((x, r)\) is empty for these cases.

Hence we have proved Theorem 3.1.

Proof of Theorem 3.2:

As in the case of Theorem 3.1, we have \( b - b_0 = mx \) where \( x \) is an integer when \((m - 1)r\) is even and it is an odd positive multiple of 1/2 when \((m - 1)r\) is odd. Substituting \( mx \) for \( b - b_0 \) in (3.1) gives us the expression in (A.1). We now consider each of the cases.

(1) Here we have \( m \) even and \( 1/2 \leq (b - 2)/m \leq t \). We consider four subcases.

Suppose \( r \) is an odd integer in the interval

\[
\max \left\{ 0, \frac{2(m - b + 2)}{m(m - 1)} \right\} \leq r \leq \frac{2(mt - b + 2)}{m(m - 1)}.
\]  

(A.2)

Then \( x \) must be an odd positive multiple of 1/2. The expression in (A.1) is minimized with respect to \( x \) by choosing \( x \) to be as large as possible within its range of allowable values. It is easy to verify that \( x \) cannot exceed \((b - 2)/m\) under this case, so we choose \( x \) to be the largest odd positive multiple of 1/2 that is less than or equal to \((b - 2)/m\). Call this value \( x_0 \). We substitute \( x = x_0 \) in (A.1) and minimize the resulting expression with respect to \( r \). Since \( \phi \) is positive, we must pick \( r \) to be as large as possible. So \( r \) is chosen to be equal to \( r_0 \), the largest odd positive integer in the interval in (A.2).

Suppose \( r \) is an even integer in the interval in (A.2). Then \( x \) must be a positive integer. The expression in (A.1) is minimized with respect to \( x \) by choosing \( x \) to be as large as possible within its range of allowable values. Under this subcase, we must then pick \( x \) to be the largest integer, say \( x_0 \), less than or equal to \((b - 2)/m\). We substitute \( x = x_0 \) in (A.1) and minimize the resulting expression with respect to \( r \). Again, we must pick \( r \) as large as possible. So we chose \( r = r_0 \), the largest even nonnegative integer in the interval in (A.2).
Suppose $r$ is an odd integer in the interval
\[ \frac{2(mt - b + 2)}{m(m - 1)} < r \leq \frac{2(mt - 1)}{m(m - 1)}. \] \hspace{1cm} (A.3)

Then $x$ is an odd positive multiple of $1/2$ within its range of allowable values. It is easily verified that we must choose $x$ to be equal to $x_0$ where $x_0$ is given by $x_0 = t - (m - 1)r/2$. We then substitute $x = x_0$ in (A.1) and minimize the resulting expression with respect to $r$. By examining the first derivative of this expression with respect to $r$ it can be verified that it is increasing for values of $r$ in the interval in (A.3). So we choose $r$ to be the smallest odd integer, say $r_0$, in the interval given in (A.3). This leads to a design for which $r = r_0$ and $b_0 = b - mt + m(m - 1)r_0/2$.

Suppose $r$ is an even integer in the interval in (A.3). Then $x$ must be a positive integer within its range of allowable values. Again this leads to the choice $x = x_0$ where $x_0$ is $t - (m - 1)r/2$. Substituting this value for $x$ in (A.1) and minimizing with respect to $r$ leads to the choice $r = r_0$ where $r_0$ is the smallest even integer in the interval in (A.3).

By examining the best designs obtained for the above four subcases we choose the overall best design when $m$ is an even integer with $1/2 \leq (b - 2)/m \leq t$. This proves part (1) of Theorem 3.2.

Suppose $m$ is odd and $1 \leq (b - 2)/m \leq t$. Here we consider two subcases. For values of $r$ in the interval in (A.2) $x$ must be the largest positive integer, say $x_0$, less than or equal to $(b - 2)/m$. Then $r$ must be the largest integer, say $r_0$, in the interval in (A.2). For values of $r$ in the interval in (A.3) $x$ must be equal to $x_0$ where $x_0$ is the value $t - (m - 1)r/2$. Then $r$ must be the smallest integer in the interval in (A.3) because the trace can be shown to be a nondecreasing function of $r$ for values of $r$ in the interval in (A.3).

Putting the two subcases together we obtain the result in part (2) of Theorem 3.2.

For case (3) of Theorem 3.2, we have $(b - 2)/m > t$. Here $x$ must be chosen as $x_0 = t - (m - 1)r/2$. We substitute this expression for $x$ in (A.1) and note that the resulting expression is a nondecreasing function of $r$ for all allowable values of $r$. So we pick the smallest possible value of $r$, i.e., we choose $r = 0$. Hence $x = t$ and $b_0 = b - mt$.

It is easy to verify that a balanced design does not exist in the remaining cases. This concludes the proof of Theorem 3.2.