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Robust balanced measurement designs when errors are serially correlated

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Abstract

This paper considers the situation in which some characteristic is to be measured on each of several specimens. For instance, it may be the concentration of lead or arsenic in water or soil samples and a laboratory may routinely analyze samples from different sources. In the measurement process, there may be some serial correlation among measurement errors, but it is hard to detect or to have a reliable estimation for this existing phenomenon. Therefore, it may be desired to make statistical inference on the true values of unknown specimens without estimating this possible correlation. To help adjust the instrument readings in a process, standards are frequently interspersed among unknown specimens at appropriate intervals. A systematic method of arranging the order of the measurements of unknown specimens and standards is provided. One is able to avoid the difficulty of estimating the possible correlation and still has good estimates of the parameters of interest using the proposed measurement designs. In addition, a simulation study is carried out to evaluate the sensitivity of the measurement designs, showing that they are robust to the existence of various error processes.

Keywords: Calibration problem; Systematic error; Random error; Design criterion

1. Introduction

The calibration of measurement procedures is commonly required in many areas. Typical application situations include industrial processes where product quality needs to be routinely monitored and measurement laboratories where customer specimen are measured on a daily basis. A measurement process is subject to errors which may be generally classified as random errors only or a combination of both random errors and systematic errors. Here *random errors* are defined to have a zero expected value and *systematic errors* are defined to be due to biases in the measurement process. In a typical measurement process, *standards*, which have known true values traceable to a national standards laboratory (e.g. NIST in the United States), are frequently used to monitor the errors. In other words, one is capable of observing the errors whenever a standard is measured. Furthermore, in common practice, the random errors are usually assumed to be independent random variables, but it is often more realistic to acknowledge that the measurement process is serially correlated. However, it may be hard to detect this kind of serial correlation when it is weak or to have a good estimate for it when the number of standards measured is small. The main interest of this study is to develop a

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systematic approach to arranging the order of measurements so that one is able to make accurate statistical inference on the unknowns even without reliable estimates of the serial correlation.

The calibration problems for estimation procedures have been extensively studied. The reader is referred to the textbooks of Fuller (1987) and Brown (1993). But, the issues related to the order of measurements in a calibration process are rarely discussed in the literature. Earlier literature pertaining to the *measurement design*, particularly regarding the arrangement of the order of measurements, can be found in Pepper (1973) and Perng and Tong (1977). More recently, Liao et al. (2000) consider A-optimal balanced measurement designs for an additive model under the assumption that random errors arise from a first-order autoregressive process (AR(1)).

Zhou (2001) presents a design criterion for evaluation of the robustness to possible correlation among observations in general experiments. In the same paper, the criterion has been only proven successful in estimating the slope of the simple linear regression by a simulation study. Moreover, Zhou (2001) discusses the construction of robust run order for two-level factorial designs based on the criterion, but the robustness property of the obtained designs has not been thoroughly investigated. However, her work motivates us to explore applicability of the design criterion to measurement processes.

The rest of the article is organized as follows. Section 2 first introduces the design criterion presented by Zhou (2001). Then the problem of interest in this study is formulated based on this criterion. Section 3 develops an exhaustive search method for the robust balanced measurement designs. Some practical designs are also reported. Section 4 includes a simulation study for investigating robustness of the obtained designs to various autocorrelation structures. Concluding remarks are presented in Section 5.

2. Design criterion and the problem of interest

Zhou (2001) proposes an experimental design criterion for evaluation of the robustness to possible correlation among the observations. Suppose the design model of interest is assumed to be

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\boldsymbol{\beta}$ is the unknown parameters vector whose OLSE (ordinary least squares estimator) is $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$. The random errors $\boldsymbol{\epsilon}$ are serially correlated with covariance matrix $Var(\boldsymbol{y}) = \sigma^2\boldsymbol{P}$ for some correlation matrix $\boldsymbol{P}$. Without knowing $\boldsymbol{P}$, one may intend to use the OLSE for $\boldsymbol{\beta}$. Let d be the design used. The proposed criterion is based on the *change of variance function*, abbreviated as CVF, given by

$$\mathrm{CVF}_{\boldsymbol{a}}(d, \boldsymbol{P}) = \frac{\boldsymbol{a}'[V(\boldsymbol{P}) - V(\boldsymbol{I})]\boldsymbol{a}}{\boldsymbol{a}'V(\boldsymbol{I})\boldsymbol{a}}, \tag{2.1}$$

where $\boldsymbol{a}'\boldsymbol{\beta}$ is the parameter of interest; $V(\boldsymbol{P})$ is the covariance matrix of the $\hat{\boldsymbol{\beta}}$ under the assumption that $Var(\boldsymbol{y}) = \sigma^2\boldsymbol{P}$. That is,

$$Var(\hat{\boldsymbol{\beta}}) = V(\boldsymbol{P}) = \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{P}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}. \tag{2.2}$$

Moreover, $V(\boldsymbol{I}) = \sigma^2(\boldsymbol{X}'\boldsymbol{X})^{-1}$ is the covariance matrix of $\hat{\boldsymbol{\beta}}$ assuming homogeneous variances. Then the robust run order design with respect to $\boldsymbol{P}$, denoted by d^*, is defined as the design minimizing $|\mathrm{CVF}_{\boldsymbol{a}}(d, \boldsymbol{P})|$, the absolute value of the CVF, among all possible competing designs. When multiple parameters are of interest, say $\boldsymbol{a}_1'\boldsymbol{\beta}, \boldsymbol{a}_2'\boldsymbol{\beta}, \ldots, \boldsymbol{a}_k'\boldsymbol{\beta}$, the criterion is modified as

$$d^* = \min_d \sum_{i=1}^{k} |\mathrm{CVF}_{\boldsymbol{a}_i}(d, \boldsymbol{P})|. \tag{2.3}$$

Zhou (2001) also suggests that it may be reasonable to assume MA(1), a first-order moving average, error process in construction of the robust designs for practical use.

In this study, we are interested in determining robust measurement designs when the response variable obeys the following model

$$z_i = \mu + \delta_{i,0}\tau_0 + \sum_{j=1}^{m} \delta_{i,j}\tau_j + \varepsilon_i, \tag{2.4}$$