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Design of linear calibration experiments

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ABSTRACT

This paper discusses the design of calibration experiments, focusing on approaches that minimise the uncertainties associated with the use of the instrument. For this problem, the optimal design depends on the actual response of the system and so cannot be implemented without prior information about the actual response. We review some of the standard approaches in optimal design applied to calibration problems and then consider how they can be extended to optimise the in-use uncertainty. We also consider issues when the model for the calibration function is only partially known.

1. Introduction

Calibration is a central activity in metrology and it therefore is important that calibration experiments, i.e., experiments to determine the actual response of a measuring system, are well designed [1,4]. This paper discusses linear models for calibration functions. Thus, we assume that the response of the system is modelled as

$$f(x,\boldsymbol{a}) = \sum_{j=1}^{n} a_j b_j(x), \tag{1}$$

a linear combination of basis functions $b_j(x)$ such as polynomials. If the calibration experiment produces data points (z_i,y_i), $i = 1,\ldots,m$, where the $\boldsymbol{z} = (z_1,\ldots,z_m)^T$ are known accurately, e.g., associated with accurately calibrated standards, and the measured values $\boldsymbol{y} = (y_1,\ldots,y_m)^T$ of the response are modelled as

$$y_i|\boldsymbol{a}, z_i \sim \mathrm{N}(f(z_i,\boldsymbol{a}),\sigma^2),$$

then the best estimates of the calibration parameters are given by

$$\hat{\boldsymbol{a}} = (C^TC)^{-1}C^T\boldsymbol{y},$$

and the variance matrix associated with these estimates is given by

$$V = V(\boldsymbol{z}) = \sigma^2(C^TC)^{-1},$$

where C is the observation matrix with $C_{ij} = b_j(z_i)$. The variance matrix $V = V(\boldsymbol{z})$ depends on the design of the calibration experiment through $\boldsymbol{z}$.

If C has QR factorisation [2]

$$C = QR = [\,Q_1 \quad Q_2\,]\begin{bmatrix} R_1 \\ \boldsymbol{0} \end{bmatrix} = Q_1R_1, \tag{2}$$

where Q is an $m \times m$ orthogonal matrix and R is an $m \times n$ upper triangular matrix with Q_1, Q_2 and R_1 determined by partitioning Q and R, then

$$\hat{\boldsymbol{a}} = R_1^{-1}Q_1^T\boldsymbol{y}, \quad V = \sigma^2\left(R_1^TR_1\right)^{-1}.$$

The optimality of the design is determined using criteria relating to the variance matrix V associated with the fitted parameters and information that can be derived from V. In Section 2, we consider criteria that involve only V, while in Section 3, we consider measures that relate to the uncertainties in the use of the instrument. In Section 4, we describe weighted calibration experiments. Such experiments provide an optimisation framework to determine optimal designs. Section 5 addresses the design of a calibration experiment when the model for the response is known, while Section 6 extends to the case where the response is only partially known, *a priori*. Our concluding remarks are given in Section 7.

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2. Measures of optimality based on V alone

A common approach to optimising the experimental design is to minimise some aggregate measure of uncertainty based on $V(\boldsymbol{z})$. For example, the A-optimality criterion seeks to choose $\boldsymbol{z}$ so as to minimise the trace

$$\mathrm{Tr}(V) = \sum_{j=1}^{n} v_{jj} = \sum_{j=1}^{n} \lambda_j,$$

the sum of the diagonal elements of $V = V(\boldsymbol{z})$ which is equal to the sum of the eigenvalues λ_j of V. The D-optimality criterion seeks to minimise the determinant $|V| = \prod_{j=1}^{n} \lambda_j$ of V, i.e., minimise the product of the eigenvalues of V. The E-optimality criterion seeks to minimise the maximum eigenvalue of V while T-optimality seeks to maximise $\sum_{j=1}^{n} \frac{1}{\lambda_j}$.

The D-optimality criterion has the important property of being invariant with respect to changes in parametrization. For example, if the calibration function is described as a polynomial, then a number of basis functions can be used. The monomial basis functions $b_j(x) = x^j$, $j \geqslant 0$ are often used but this choice can lead to numerical difficulties for higher degree polynomials. As an alternative, Chebyshev polynomial basis functions $T_j(x)$ have very good numerical properties. For $-1 \leqslant x \leqslant 1$, the basis functions are defined by

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x), \quad j \geqslant 2.$$

(In practice $T_0(x)$ is replaced by $T_0(x)/2$ in the set of basis functions.) If $\tilde{\boldsymbol{a}}$ represents the new (linear) parametrization, related to the old parametrization by $\boldsymbol{a} = J\tilde{\boldsymbol{a}}$ and $\widetilde{C} = CJ$ is the observation matrix associated with $\tilde{\boldsymbol{a}}$, then the corresponding variance matrix $\widetilde{V}$ is given by

$$\widetilde{V} = \sigma^2(\widetilde{C}^T\widetilde{C})^{-1} = \sigma^2 J^{-1}(C^TC)^{-1}J^{-T} = J^{-1}VJ^{-T},$$

and

$$|\widetilde{V}| = |J|^{-2}|V|,$$

so minimising $|\widetilde{V}|$ is the same as minimising $|V|$, since J does not depend on the design.

For the above criteria, determining the optimal design amounts to minimising some utility measure $E(\boldsymbol{z})$ with respect to $\boldsymbol{z}$ where the utility measure does not depend on the shape of the response function as specified by $\boldsymbol{a}$.

3. Measures relating to the in-use uncertainty

An instrument is calibrated in order that measurements made by the instrument are traceable and can be assigned valid uncertainties. Given a measured response y, we wish to determine an estimate of x, the stimulus that gave rise to the response, along with its associated uncertainty. The uncertainties associated with the calibration parameters $\boldsymbol{a}$ contribute to the in-use uncertainty but it is not the only source of uncertainty. Suppose the calibration parameters are estimated by $\hat{\boldsymbol{a}}$ with associated variance matrix $V = V(\boldsymbol{z})$. Given a measured response, modelled as

$$y|\boldsymbol{a}, x \in \mathrm{N}(f(x,\boldsymbol{a}), \sigma^2), \tag{3}$$

the estimate $\hat{x}$ of x is such that $y = f(\hat{x}, \hat{\boldsymbol{a}})$. The uncertainty associated with this estimate is

$$u^2(\hat{x}) = u^2(\hat{x}, \boldsymbol{z}, \hat{\boldsymbol{a}}) = \frac{\sigma^2 + \boldsymbol{b}(\hat{x})^T V(\boldsymbol{z})\boldsymbol{b}(\hat{x})}{\dot{f}^2(\hat{x}, \hat{\boldsymbol{a}})} = \frac{\sigma^2 + u^2(f(\hat{x}, \hat{\boldsymbol{a}}))}{\dot{f}^2(\hat{x}, \hat{\boldsymbol{a}})}$$

where

$$\dot{f}(x, \boldsymbol{a}) = \frac{\partial f}{\partial x}(x, \boldsymbol{a}) = \dot{\boldsymbol{b}}^T\boldsymbol{a}, \quad \dot{b}_j = \frac{\partial b_j}{\partial x}(x, \boldsymbol{a}).$$

Thus, the in-use uncertainty depends on $V(\boldsymbol{z})$ but also on the shape of the calibration curve through $\dot{f}(x, \boldsymbol{a})$, estimated by $\dot{f}(\hat{x}, \hat{\boldsymbol{a}})$. Note that the parametrization of the model affects the measure of in-use uncertainty through terms of the form $\boldsymbol{b}^TV\boldsymbol{b}$ and, following the same argument as described for D-optimality above, these terms are invariant with respect to changes in the parametrization. Hence, the in-use uncertainty is also invariant with respect to changes in parametrization.

Let

$$u^2(x, \boldsymbol{z}, \boldsymbol{a}) = \frac{\sigma^2 + \boldsymbol{b}(x)^T V(\boldsymbol{z})\boldsymbol{b}(x)}{\dot{f}^2(x, \boldsymbol{a})}, \tag{4}$$

so that $u(x,\boldsymbol{z},\boldsymbol{a})$ represents the expected uncertainty associated with the estimate of x determined from a measurement by an instrument whose response is modelled as in (3). We wish to design the calibration experiment, i.e., choose $\boldsymbol{z}$ so that a measure of the in-use uncertainty, aggregated over the working range of the instrument, is minimised. In particular, we may wish to optimise the performance of the instrument in a particular working range, corresponding to the most common application. Let $p(x)$ be a prior density for x defined on the working range $[A,B]$, specifying the likely distribution of artefacts to be measured by the instrument and define

$$E_\infty(\boldsymbol{z}, \boldsymbol{a}) = \max_{x \in [A,B]} u(x, \boldsymbol{z}, \boldsymbol{a}), \quad E_2(\boldsymbol{z}, \boldsymbol{a}) = \int_A^B u^2(x, \boldsymbol{z}, \boldsymbol{a})p(x)dx.$$

The first aggregate measure relates to the worst performance in the working range, while the second relates to the average performance, weighted according to the prior density $p(x)$. In general terms, the design of experiment task is to

$$\begin{aligned} &\min_{\boldsymbol{z}} E(\boldsymbol{z}, \boldsymbol{a}) \\ &\text{s.t.} \quad A \leqslant z_j \leqslant B. \end{aligned} \tag{5}$$

The optimal performance of the instrument arises when $V(\boldsymbol{z})$ is zero, in which case the in-use uncertainty is

$$u_{\min}(x, \boldsymbol{a}) = \frac{\sigma}{|\dot{f}(x, \boldsymbol{a})|}.$$

By performing a very extensive calibration, we may be able to drive down the uncertainty contribution from the calibration parameters $\boldsymbol{a}$ so that their contribution is insignificant compared to that arising from σ. In practice, it will be sufficient to determine $\boldsymbol{a}$ with sufficient accuracy that their contribution is minor compared to σ.