XX IMEKO World Congress
Metrology for Green Growth
September 9–14, 2012, Busan, Republic of Korea

OPTIMAL DESIGN FOR LINEAR CALIBRATION PROBLEMS

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Abstract: This paper considers the design of instrument calibration experiments with the focus of minimising 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 consider a number of approaches.

Keywords: linear calibration, optimal design

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 [1,2,3,5]. We assume that the response of the system is modelled as

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

a linear combination of basis functions $b_j(x)$ such as polynomials. If the calibration experiment produces data points (z_i, y_i), $i = 1, \dots, m_0$, where the z_i are known accurately, e.g., associated with accurately calibrated standards, and the measured values of the response y_i are modelled as

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

then the best estimates of the calibration parameters are given by $\hat{\boldsymbol{a}} = (C^\mathrm{T}C)^{-1}C^\mathrm{T}\boldsymbol{y}$, and variance matrix associated with these estimates is given by

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

where C is the observation matrix with $C_{ij} = b_j(z_i)$. Note that V depends on the design of the calibration experiment through $\boldsymbol{z} = \left(z_1, \dots, z_{m_0}\right)^\mathrm{T}$.

2. IN-USE UNCERTAINTY

In use, if a response y is recorded, then the best estimate of the measurand x that gave rise to that response is given by the $\hat{x}$ that solves $y = f(x, \hat{\boldsymbol{a}})$. The uncertainty associated with this estimate [4] is given by

$$u^2(\hat{x}) = u^2(\hat{x}, \boldsymbol{z}, \hat{\boldsymbol{a}}) = \frac{\sigma^2 + \boldsymbol{b}(\hat{x})^\mathrm{T} V(\boldsymbol{z}) \boldsymbol{b}(\hat{x})}{\dot{f}^2(\hat{x}, \hat{\boldsymbol{a}})}, \quad (1)$$

where $\boldsymbol{b}(x) = \left(b_1(x), \dots, b_n(x)\right)^\mathrm{T}$ and

$$\dot{f}(x, \boldsymbol{a}) = \frac{\partial f}{\partial x}(x, \boldsymbol{a}) = \dot{\boldsymbol{b}}^\mathrm{T}\boldsymbol{a},$$

with $\dot{\boldsymbol{b}}(x) = \left(\dot{b}_1(x), \dots, \dot{b}_n(x)\right)^\mathrm{T}$ and

$$\dot{b}_j = \frac{db_j}{dx}.$$

From (1) we write

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

We are interested in determining $\boldsymbol{z}$ such that some measure involving $u(x, \boldsymbol{z}, \boldsymbol{a})$ is minimised.

3. UTILITY MEASURES

We consider two such measures:

$$E_\infty(\boldsymbol{z}, \boldsymbol{a}) = \max_{x \in [A,B]} u(x, \boldsymbol{z}, \boldsymbol{a}),$$

and

$$E_2(\boldsymbol{z}, \boldsymbol{a}) = \int_A^B u^2(x, \boldsymbol{z}, \boldsymbol{a})\, p(x) dx,$$

where $p(x)$ is a prior density for *x* reflecting the likely usage of the instrument. The first measure specifies a minimum level of performance for measurands in the range $[A, B]$ while the second reflects an average level of performance in that range.

3. OPTIMISATION APPROACHES

We assume that a minimal calibration has been undertaken involving *n* calibration points to determine the *n* parameters associated with the linear model. This gives rise to an initial estimate $\boldsymbol{a}_0$ of the calibration parameters with associated variance matrix V_0. We then have a minimal level of performance given by

$$u_L^2(x, \boldsymbol{a}_0) = \frac{\sigma^2 + \boldsymbol{b}(x)^\mathrm{T} V_0 \boldsymbol{b}(x)}{\dot{f}^2(x, \boldsymbol{a}_0)},$$

and a maximum level of performance in which there is no uncertainty associated with the calibration function:

$$u_U^2(x, \boldsymbol{a}_0) = \frac{\sigma^2}{\dot{f}^2(x, \boldsymbol{a}_0)}.$$

For additional calibration points, the resulting uncertainty curve will lie between these two curves. The aim is to choose the additional points so that the uncertainty curve approaches the optimal curve as quickly as possible.

This paper will discuss a number of optimization approaches a) sequential approaches in which the next calibration point is optimally chosen, and b) point density approaches in which the optimal number of repeat measurements for a finite choice of possible z_i is determined. The paper will also discuss models in which the response function includes a Gaussian processes [6] component to account for systematic but unknown behavior associated with the instrument.

4. ACKNOWLEDGEMENT

This work is supported by the UK's National Measurement Office Mathematics and Modelling for Metrology programme.

5. REFERENCES

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